



wwPDB EM Validation Summary Report ⓘ

Mar 9, 2026 – 08:27 AM UTC

PDB ID : 6BX0 / pdb_00006bx0
EMDB ID : EMD-7301
Title : Atomic resolution structure of human bufavirus 2
Authors : Mietzsch, M.; Agbandje-McKenna, M.
Deposited on : 2017-12-15
Resolution : 3.79 Å(reported)

This is a wwPDB EM Validation Summary Report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/EMValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

EMDB validation analysis : 0.0.1.dev132
MolProbity : 4-5-2 with Phenix2.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data in the EMDb archive up until May 2025)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

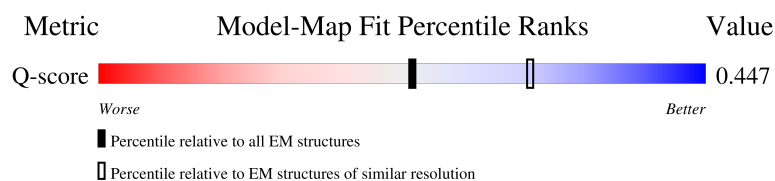
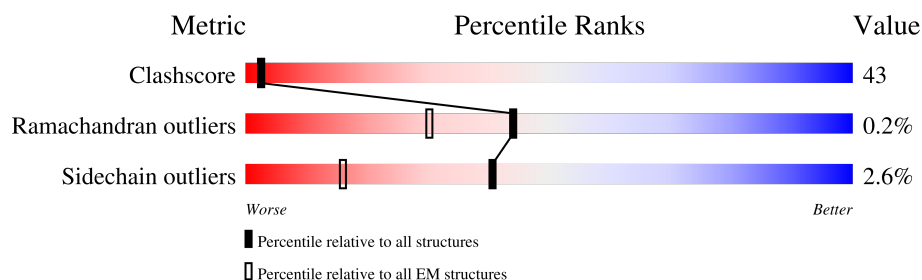
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 3.79 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
Q-score	-	25397	10018 (3.29 - 4.29)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the map. The red, orange, yellow and green segments of the bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the EM map (all-atom inclusion $< 40\%$). The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	0	537	
1	1	537	
1	2	537	
1	3	537	

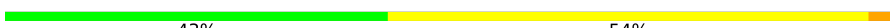
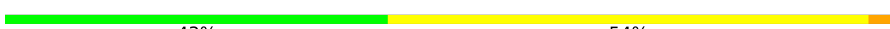
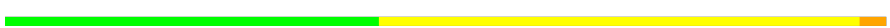
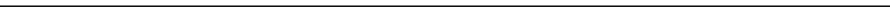
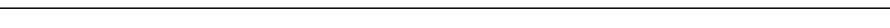
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Mol	Chain	Length	Quality of chain	
1	4	537	43%	53%
1	5	537	42%	54%
1	6	537	43%	53%
1	7	537	42%	54%
1	A	537	43%	53%
1	B	537	42%	54%
1	C	537	42%	54%
1	D	537	42%	54%
1	E	537	42%	54%
1	F	537	43%	53%
1	G	537	43%	53%
1	H	537	42%	54%
1	I	537	42%	54%
1	J	537	43%	53%
1	K	537	42%	54%
1	L	537	42%	54%
1	M	537	42%	54%
1	N	537	42%	54%
1	O	537	42%	54%
1	P	537	42%	54%
1	Q	537	42%	54%
1	R	537	43%	53%
1	S	537	43%	53%
1	T	537	43%	53%
1	U	537	43%	53%

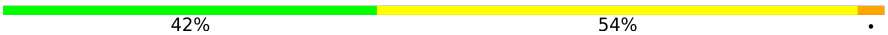
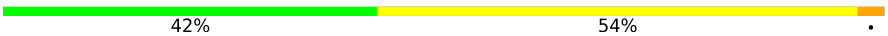
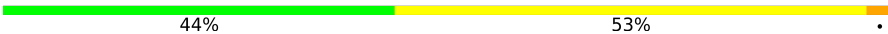
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Mol	Chain	Length	Quality of chain	
1	V	537		.
1	W	537		.
1	X	537		.
1	Y	537		.
1	Z	537		.
1	a	537		.
1	b	537		.
1	c	537		.
1	d	537		.
1	e	537		.
1	f	537		.
1	g	537		.
1	h	537		.
1	i	537		.
1	j	537		.
1	k	537		.
1	l	537		.
1	m	537		.
1	n	537		.
1	o	537		.
1	p	537		.
1	q	537		.
1	r	537		.
1	s	537		.
1	t	537		.

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Mol	Chain	Length	Quality of chain
1	u	537	 42%54%.
1	v	537	 43%53%.
1	w	537	 44%53%.
1	x	537	 42%54%.
1	y	537	 42%54%.
1	z	537	 44%53%.

2 Entry composition

There is only 1 type of molecule in this entry. The entry contains 259560 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called VP2.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	535	Total	C	N	O	S	0	0
			4326	2727	763	817	19		
1	B	535	Total	C	N	O	S	0	0
			4326	2727	763	817	19		
1	C	535	Total	C	N	O	S	0	0
			4326	2727	763	817	19		
1	D	535	Total	C	N	O	S	0	0
			4326	2727	763	817	19		
1	E	535	Total	C	N	O	S	0	0
			4326	2727	763	817	19		
1	F	535	Total	C	N	O	S	0	0
			4326	2727	763	817	19		
1	G	535	Total	C	N	O	S	0	0
			4326	2727	763	817	19		
1	H	535	Total	C	N	O	S	0	0
			4326	2727	763	817	19		
1	I	535	Total	C	N	O	S	0	0
			4326	2727	763	817	19		
1	J	535	Total	C	N	O	S	0	0
			4326	2727	763	817	19		
1	K	535	Total	C	N	O	S	0	0
			4326	2727	763	817	19		
1	L	535	Total	C	N	O	S	0	0
			4326	2727	763	817	19		
1	M	535	Total	C	N	O	S	0	0
			4326	2727	763	817	19		
1	N	535	Total	C	N	O	S	0	0
			4326	2727	763	817	19		
1	O	535	Total	C	N	O	S	0	0
			4326	2727	763	817	19		
1	P	535	Total	C	N	O	S	0	0
			4326	2727	763	817	19		
1	Q	535	Total	C	N	O	S	0	0
			4326	2727	763	817	19		

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Mol	Chain	Residues	Atoms					AltConf	Trace
1	R	535	Total 4326	C 2727	N 763	O 817	S 19	0	0
1	S	535	Total 4326	C 2727	N 763	O 817	S 19	0	0
1	T	535	Total 4326	C 2727	N 763	O 817	S 19	0	0
1	U	535	Total 4326	C 2727	N 763	O 817	S 19	0	0
1	V	535	Total 4326	C 2727	N 763	O 817	S 19	0	0
1	W	535	Total 4326	C 2727	N 763	O 817	S 19	0	0
1	X	535	Total 4326	C 2727	N 763	O 817	S 19	0	0
1	Y	535	Total 4326	C 2727	N 763	O 817	S 19	0	0
1	Z	535	Total 4326	C 2727	N 763	O 817	S 19	0	0
1	0	535	Total 4326	C 2727	N 763	O 817	S 19	0	0
1	1	535	Total 4326	C 2727	N 763	O 817	S 19	0	0
1	2	535	Total 4326	C 2727	N 763	O 817	S 19	0	0
1	3	535	Total 4326	C 2727	N 763	O 817	S 19	0	0
1	4	535	Total 4326	C 2727	N 763	O 817	S 19	0	0
1	5	535	Total 4326	C 2727	N 763	O 817	S 19	0	0
1	a	535	Total 4326	C 2727	N 763	O 817	S 19	0	0
1	b	535	Total 4326	C 2727	N 763	O 817	S 19	0	0
1	c	535	Total 4326	C 2727	N 763	O 817	S 19	0	0
1	d	535	Total 4326	C 2727	N 763	O 817	S 19	0	0
1	e	535	Total 4326	C 2727	N 763	O 817	S 19	0	0
1	f	535	Total 4326	C 2727	N 763	O 817	S 19	0	0

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Mol	Chain	Residues	Atoms					AltConf	Trace
1	g	535	Total 4326	C 2727	N 763	O 817	S 19	0	0
1	h	535	Total 4326	C 2727	N 763	O 817	S 19	0	0
1	i	535	Total 4326	C 2727	N 763	O 817	S 19	0	0
1	j	535	Total 4326	C 2727	N 763	O 817	S 19	0	0
1	k	535	Total 4326	C 2727	N 763	O 817	S 19	0	0
1	l	535	Total 4326	C 2727	N 763	O 817	S 19	0	0
1	m	535	Total 4326	C 2727	N 763	O 817	S 19	0	0
1	n	535	Total 4326	C 2727	N 763	O 817	S 19	0	0
1	o	535	Total 4326	C 2727	N 763	O 817	S 19	0	0
1	p	535	Total 4326	C 2727	N 763	O 817	S 19	0	0
1	q	535	Total 4326	C 2727	N 763	O 817	S 19	0	0
1	r	535	Total 4326	C 2727	N 763	O 817	S 19	0	0
1	s	535	Total 4326	C 2727	N 763	O 817	S 19	0	0
1	t	535	Total 4326	C 2727	N 763	O 817	S 19	0	0
1	u	535	Total 4326	C 2727	N 763	O 817	S 19	0	0
1	v	535	Total 4326	C 2727	N 763	O 817	S 19	0	0
1	w	535	Total 4326	C 2727	N 763	O 817	S 19	0	0
1	x	535	Total 4326	C 2727	N 763	O 817	S 19	0	0
1	y	535	Total 4326	C 2727	N 763	O 817	S 19	0	0
1	z	535	Total 4326	C 2727	N 763	O 817	S 19	0	0
1	6	535	Total 4326	C 2727	N 763	O 817	S 19	0	0

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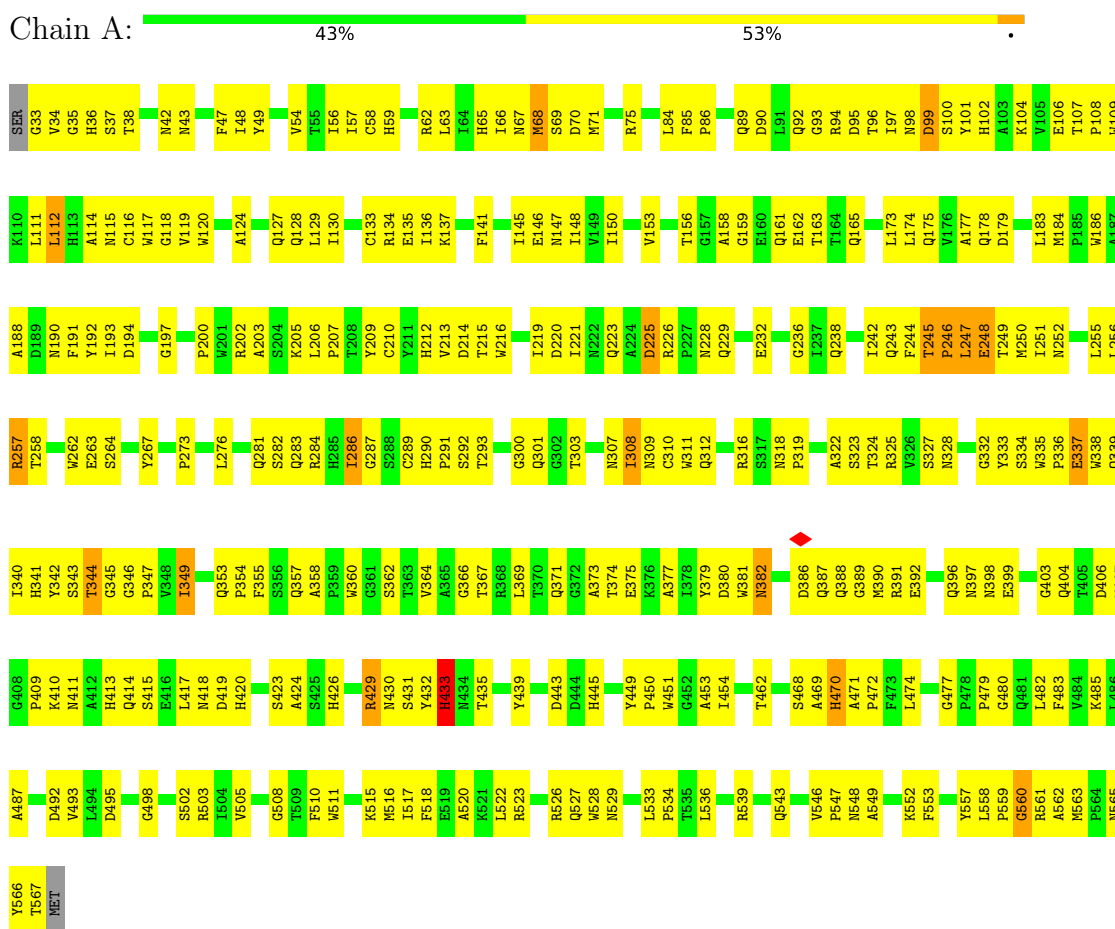
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Mol	Chain	Residues	Atoms					AltConf	Trace
1	7	535	Total	C	N	O	S	0	0
			4326	2727	763	817	19		

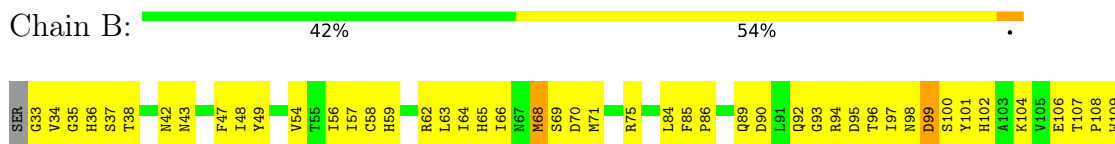
3 Residue-property plots

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion in map density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red diamond above a residue indicates a poor fit to the EM map for this residue (all-atom inclusion < 40%). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

• Molecule 1: VP2



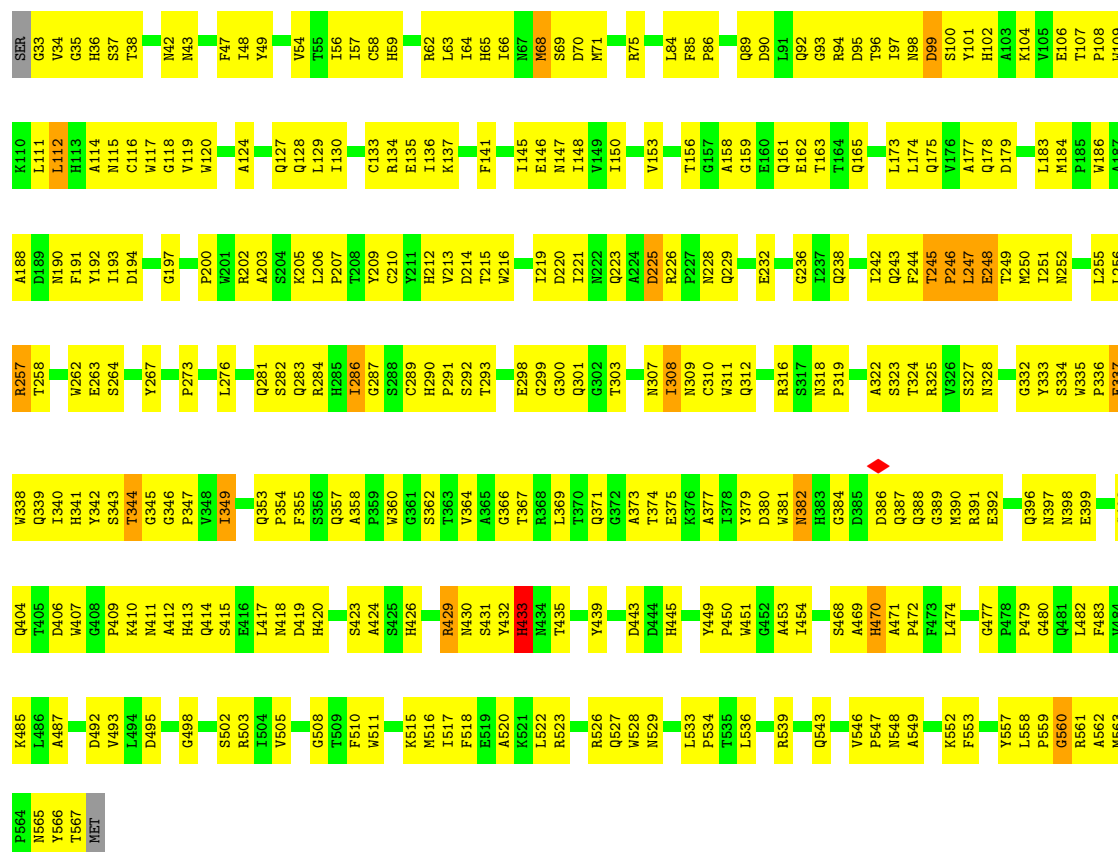
• Molecule 1: VP2



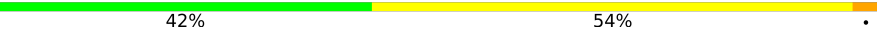


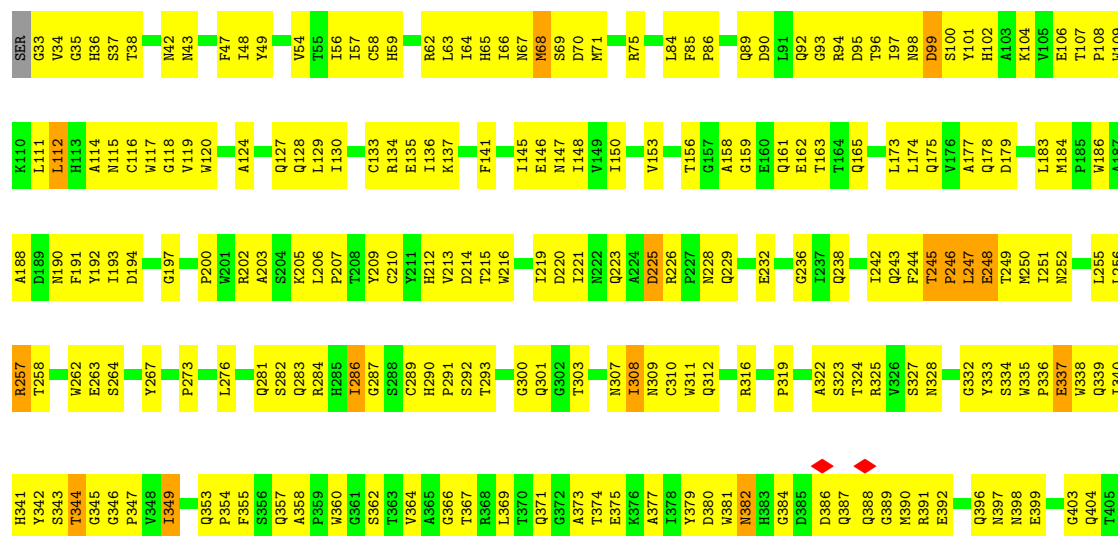
- Molecule 1: VP2

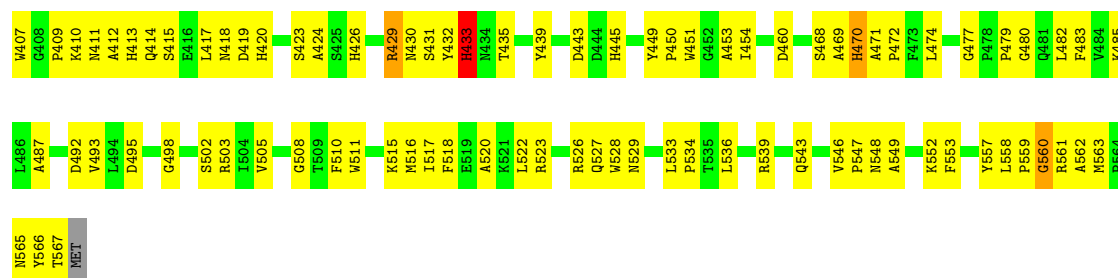
Chain D: 



- Molecule 1: VP2

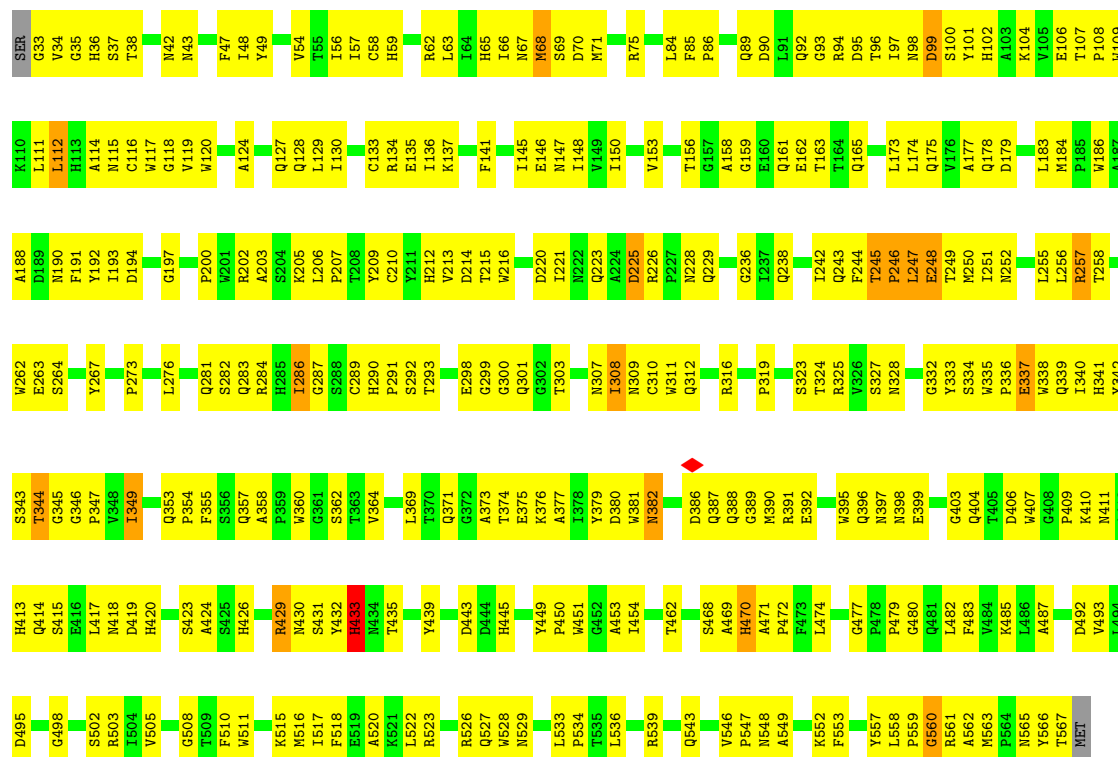
Chain E: 





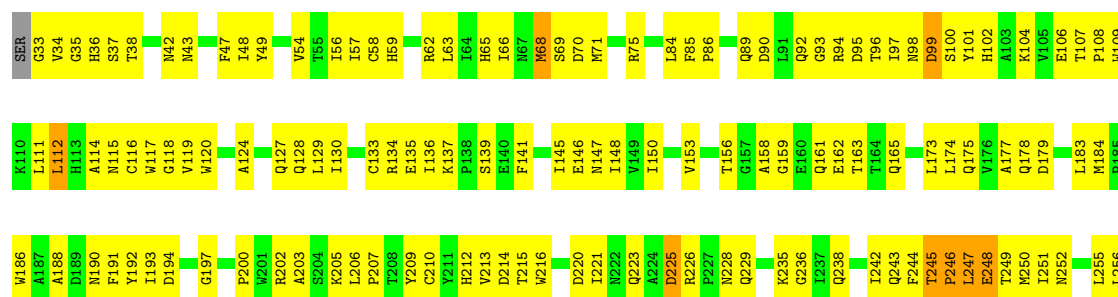
• Molecule 1: VP2

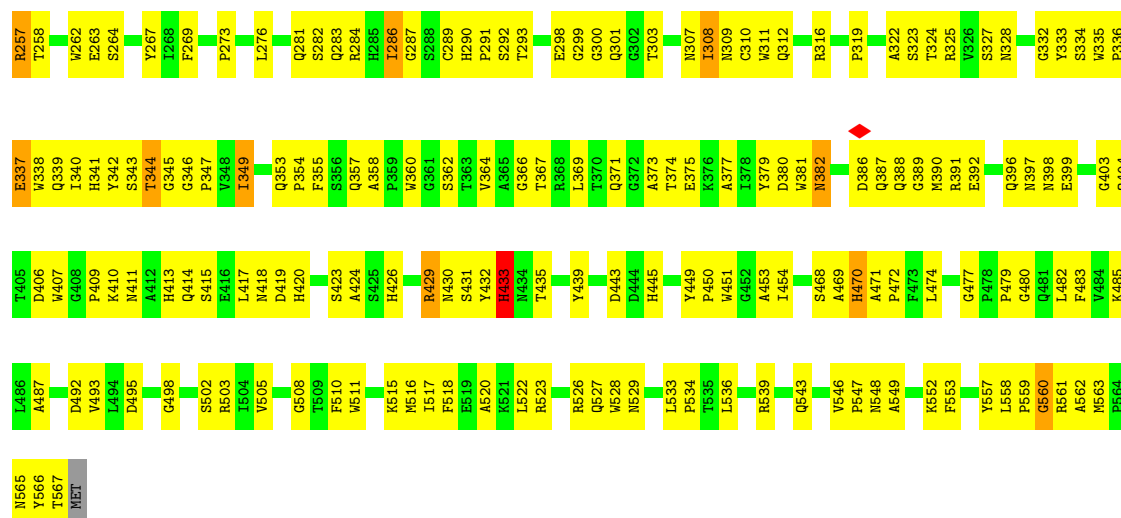
Chain F: 43% 53%



• Molecule 1: VP2

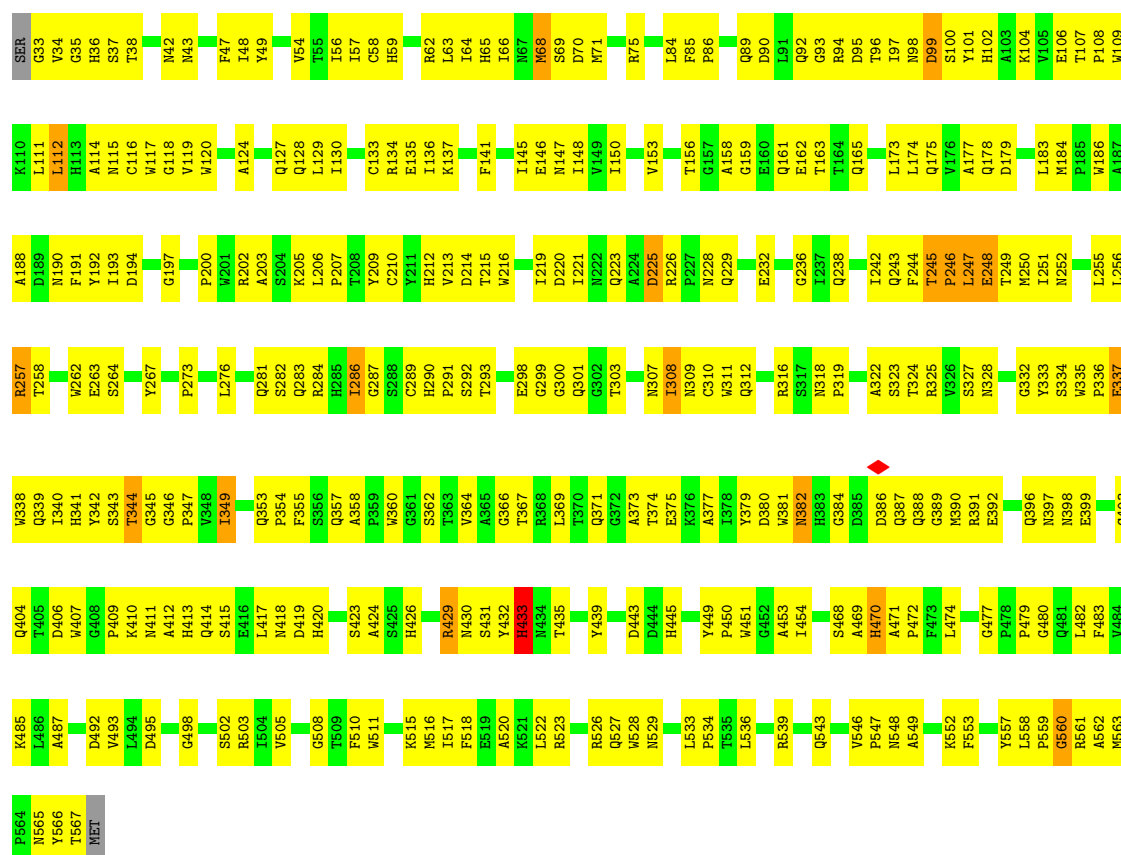
Chain G: 43% 53%





• Molecule 1: VP2

Chain H: 42% 54%



• Molecule 1: VP2

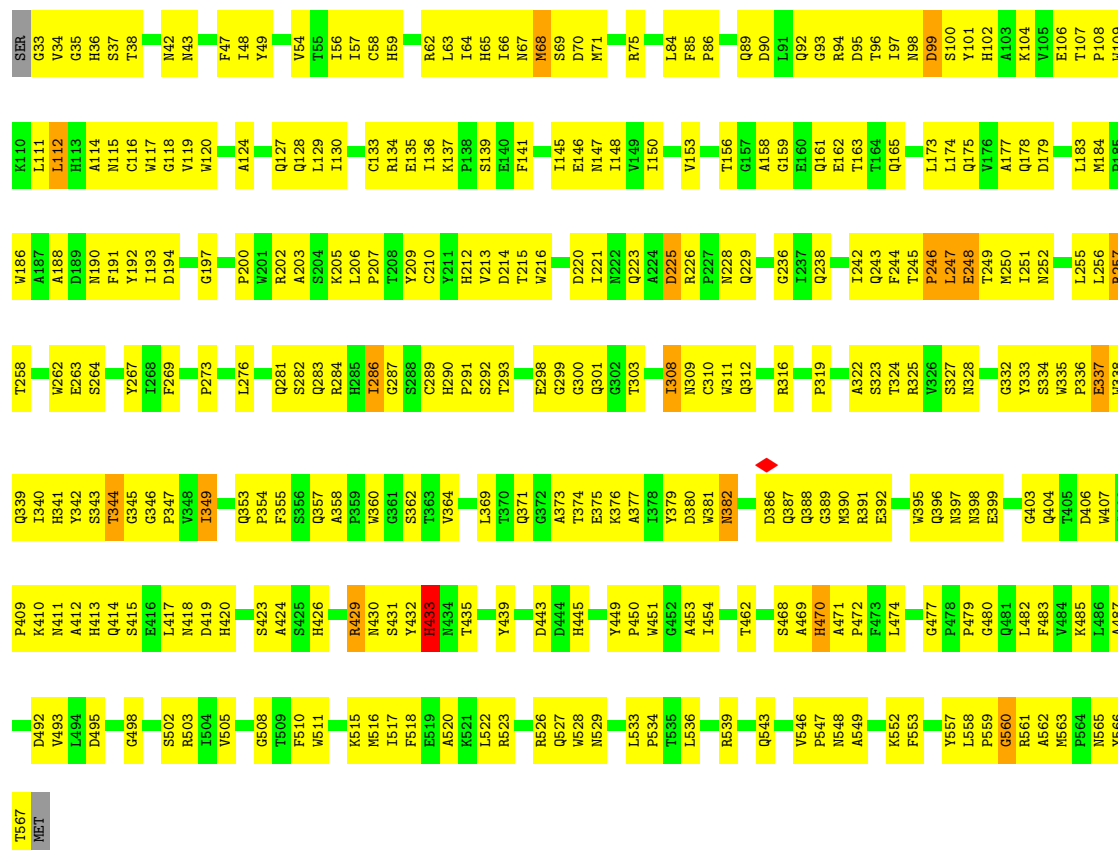
Chain I: 42% 54%





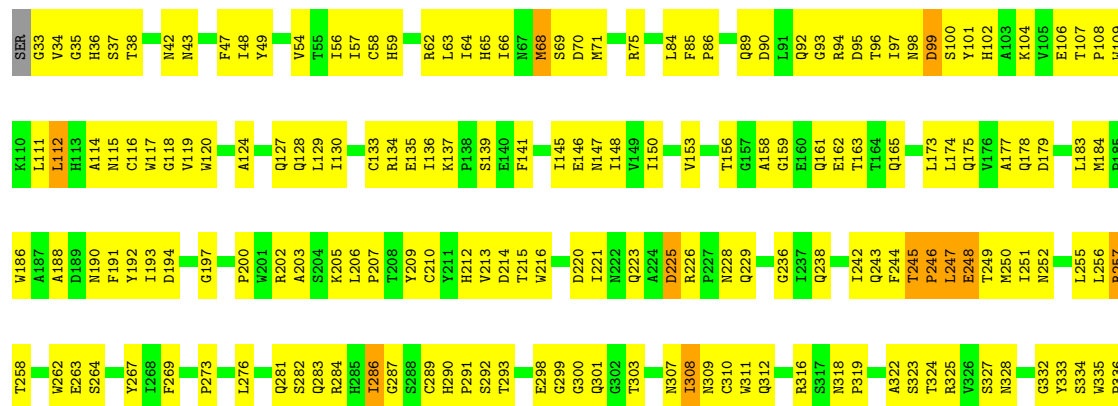
• Molecule 1: VP2

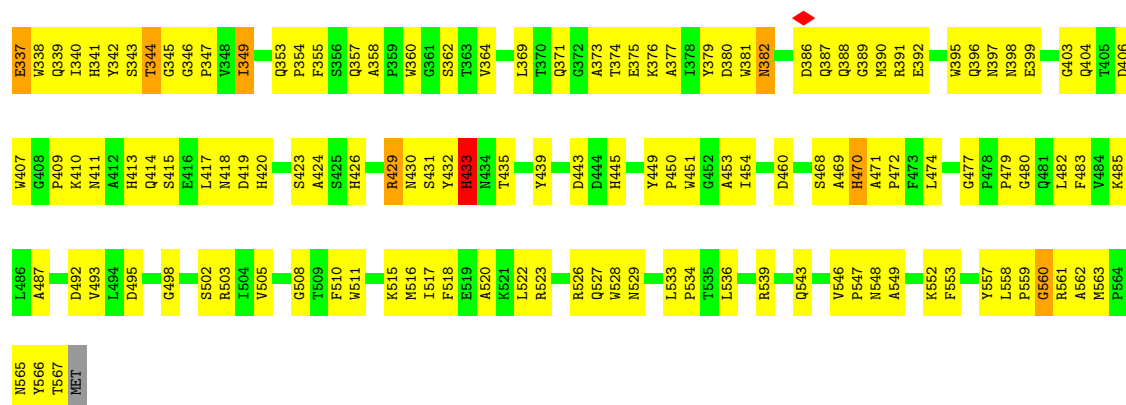
Chain K: 42% 54%



• Molecule 1: VP2

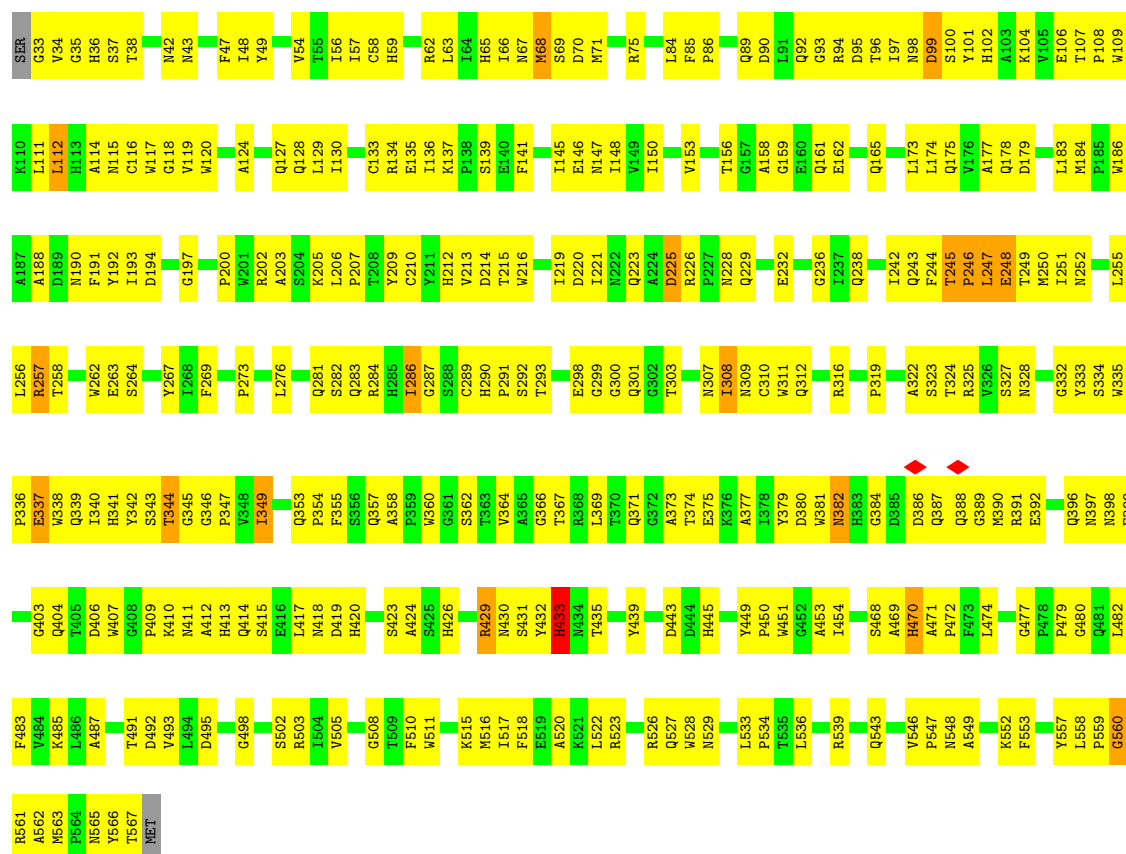
Chain L: 42% 54%





• Molecule 1: VP2

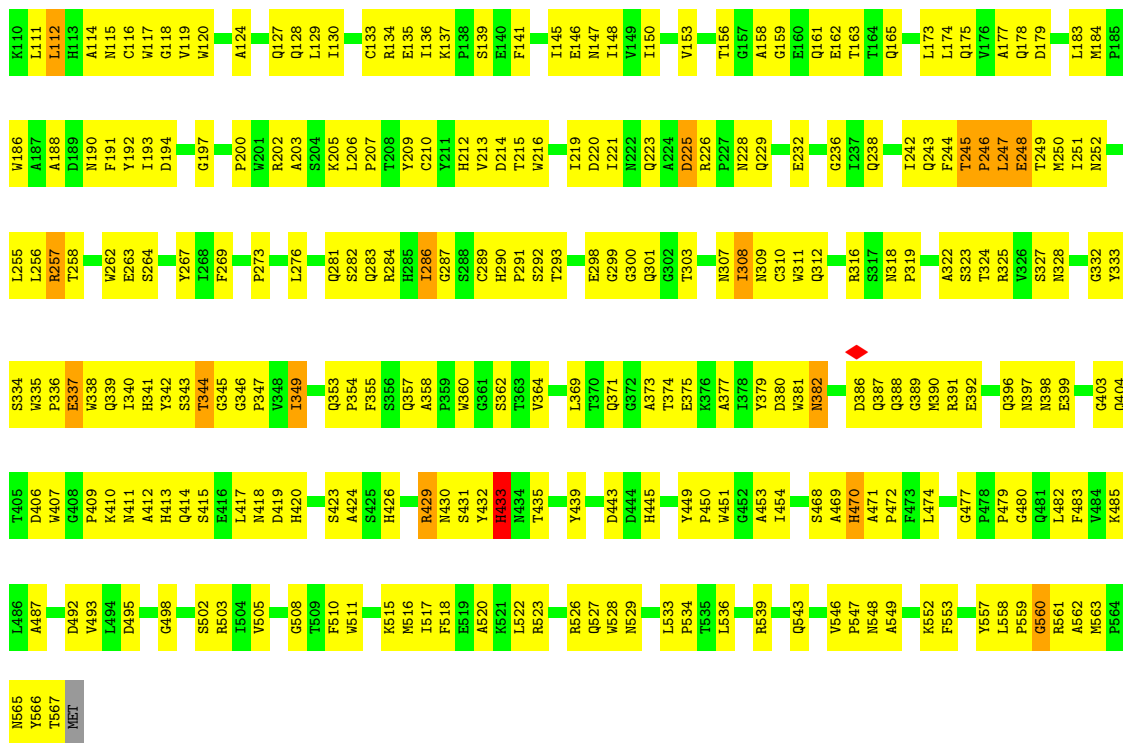
Chain M: 42% 54%



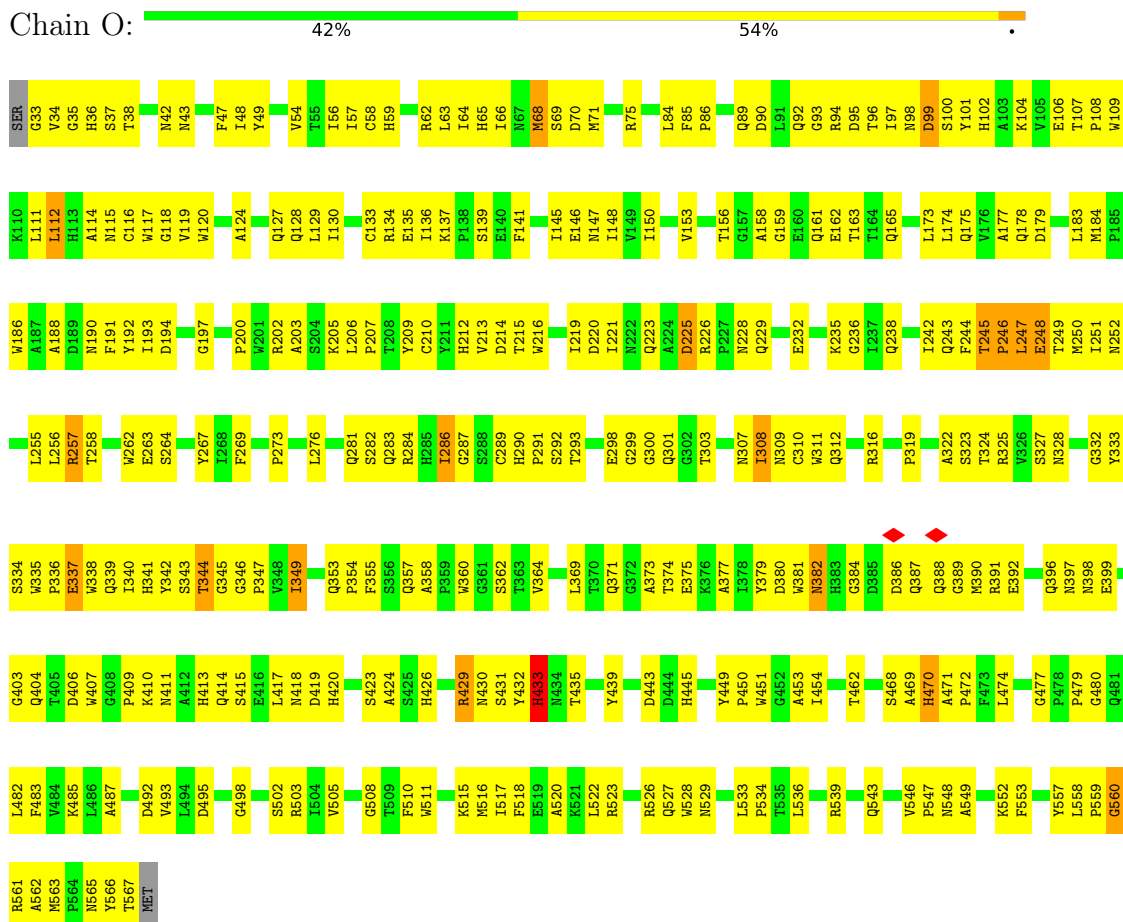
• Molecule 1: VP2

Chain N: 42% 54%



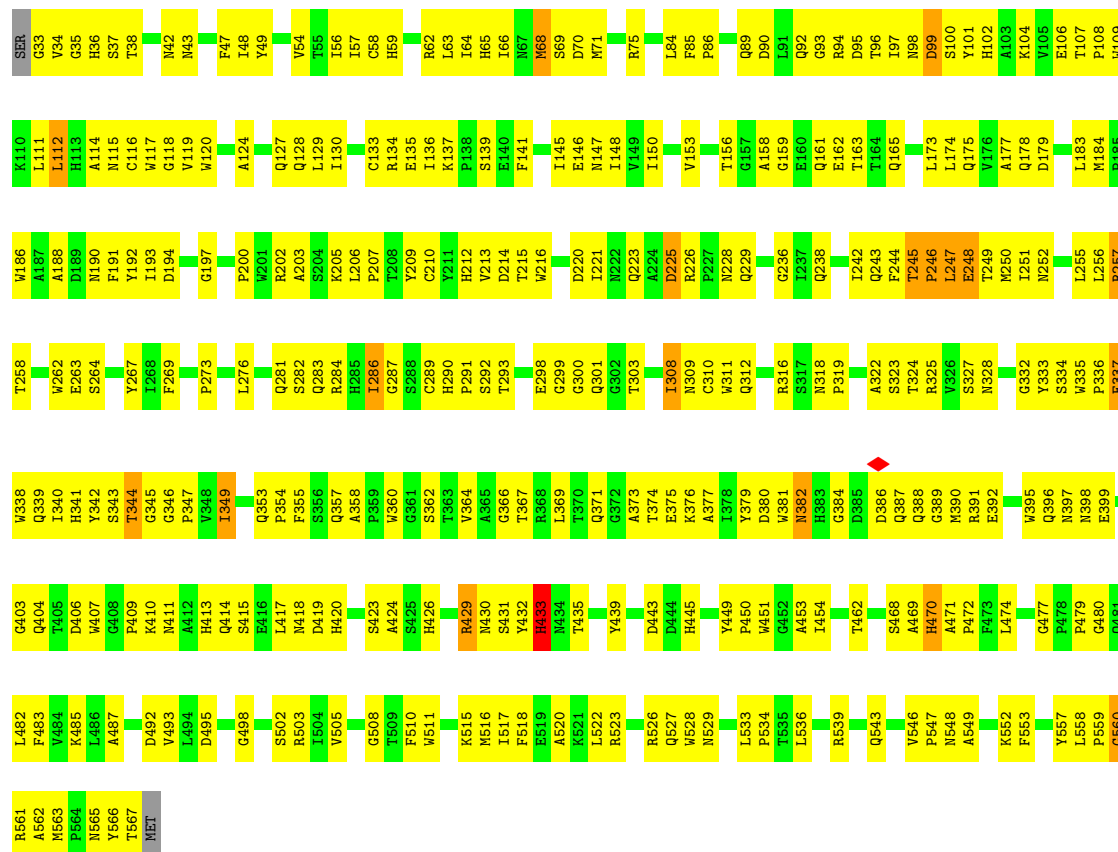


- Molecule 1: VP2



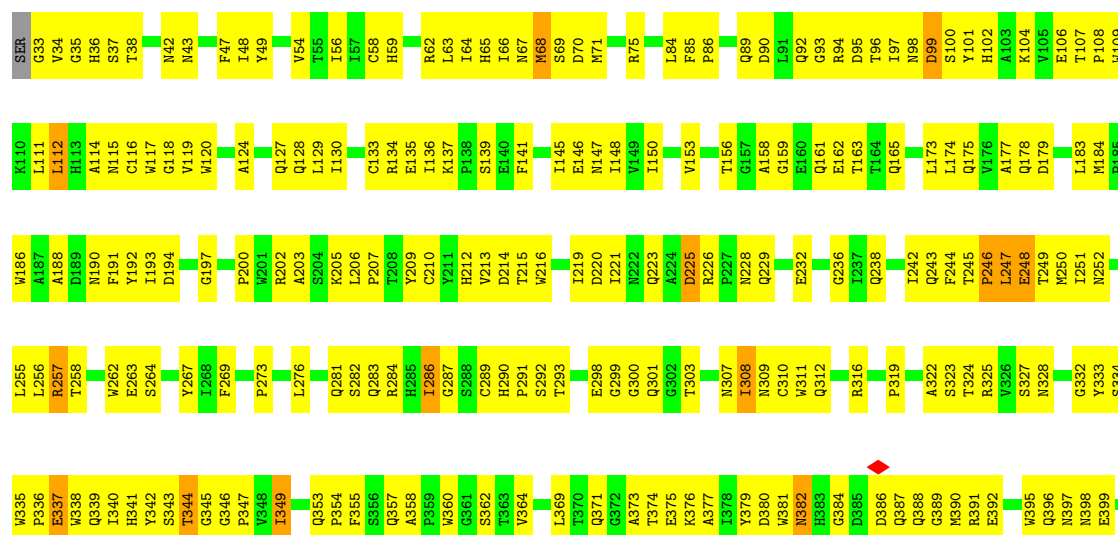
• Molecule 1: VP2

Chain P:  42% 54%

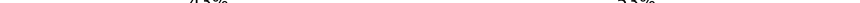


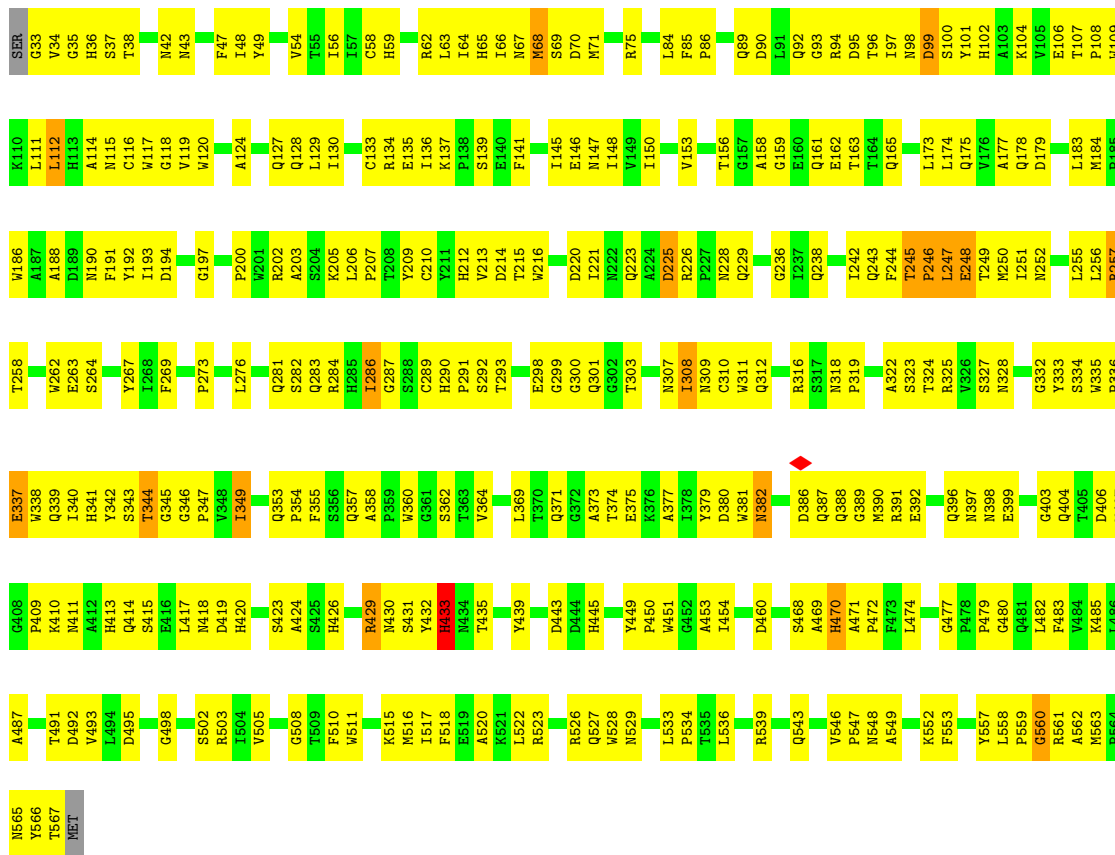
• Molecule 1: VP2

Chain Q:  42% 54%



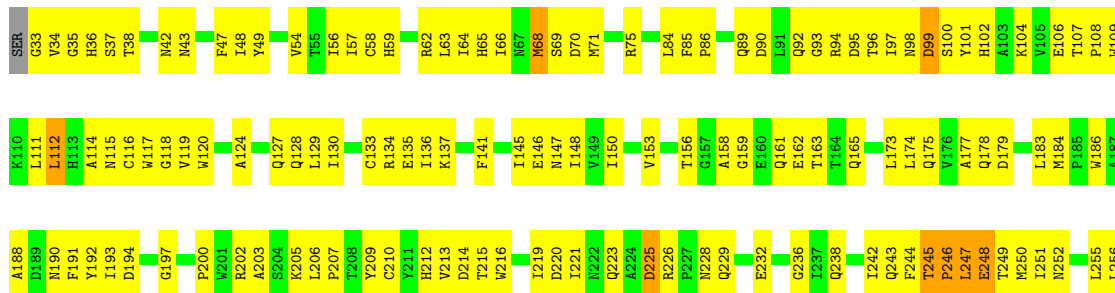
- Molecule 1: VP2

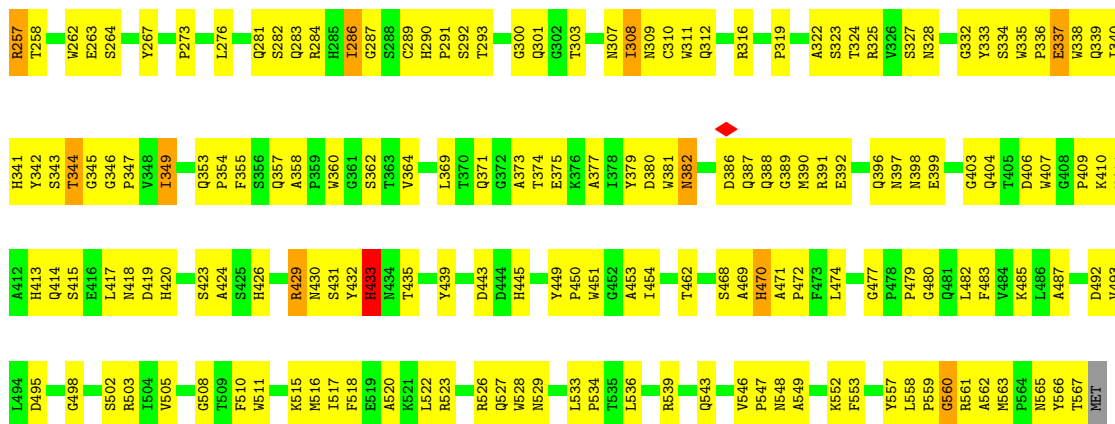
Chain R:  43% 53% .



- Molecule 1: VP2

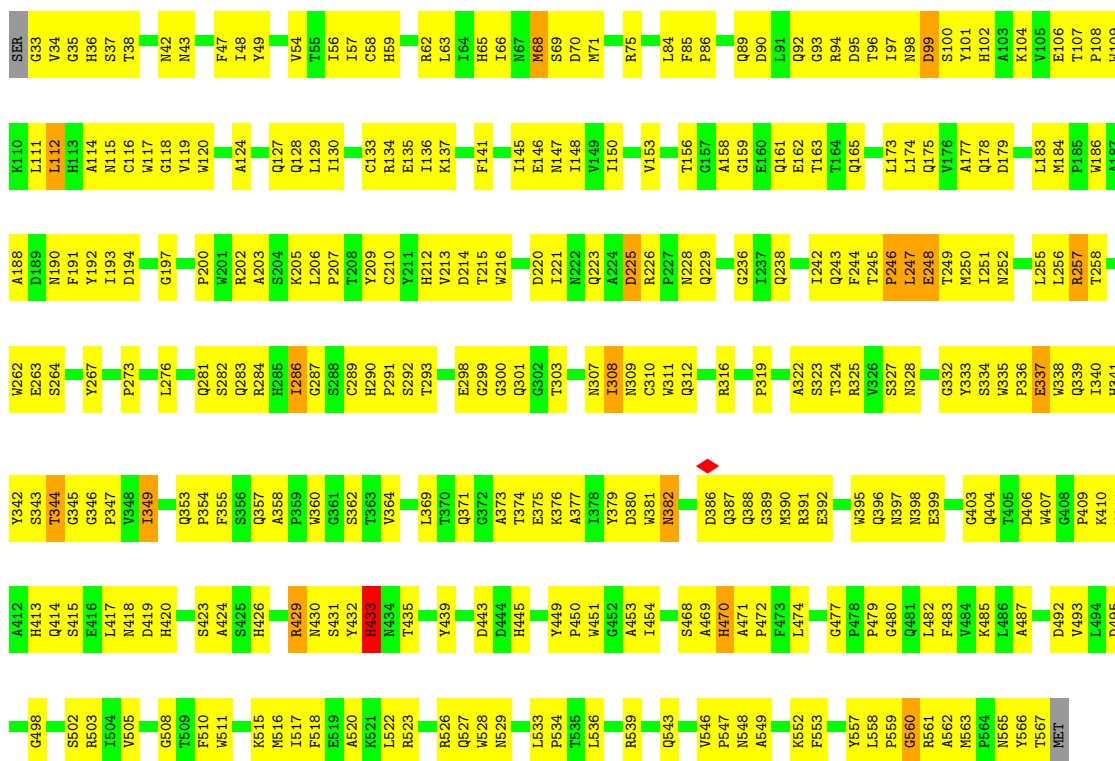
Chain S: 43% 53% .





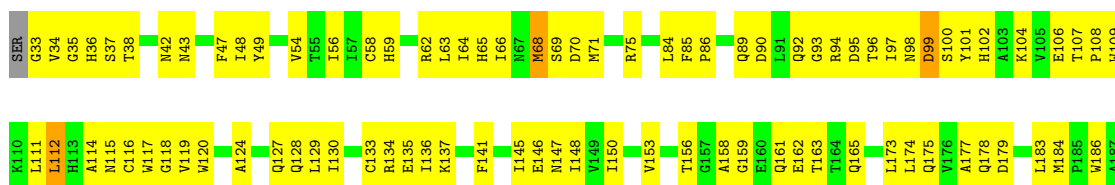
• Molecule 1: VP2

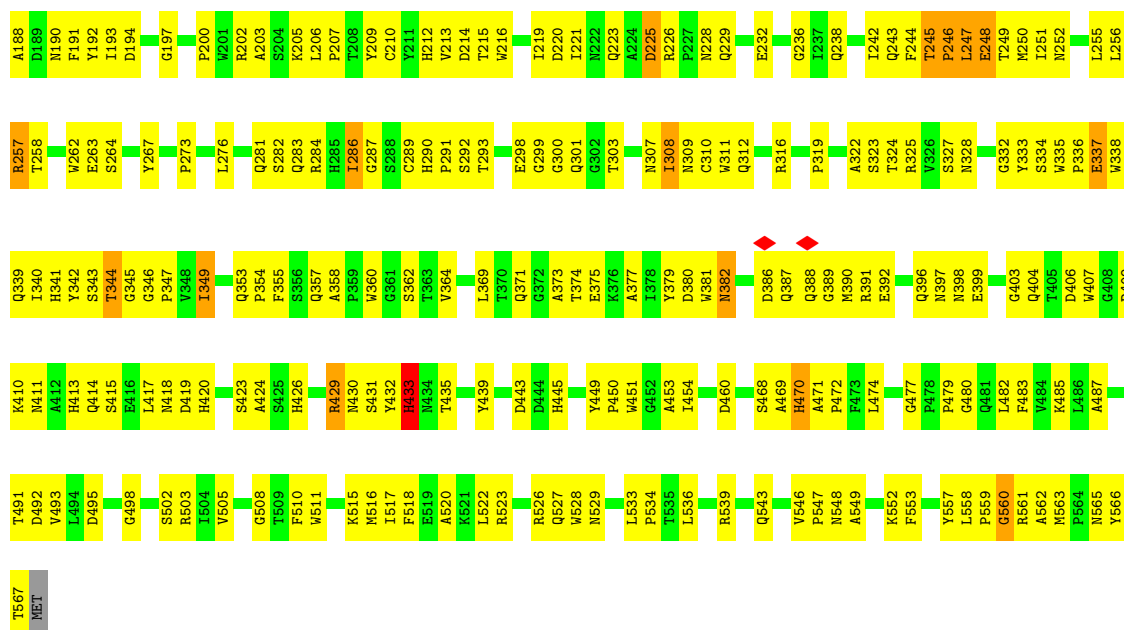
Chain T: 43% 53%



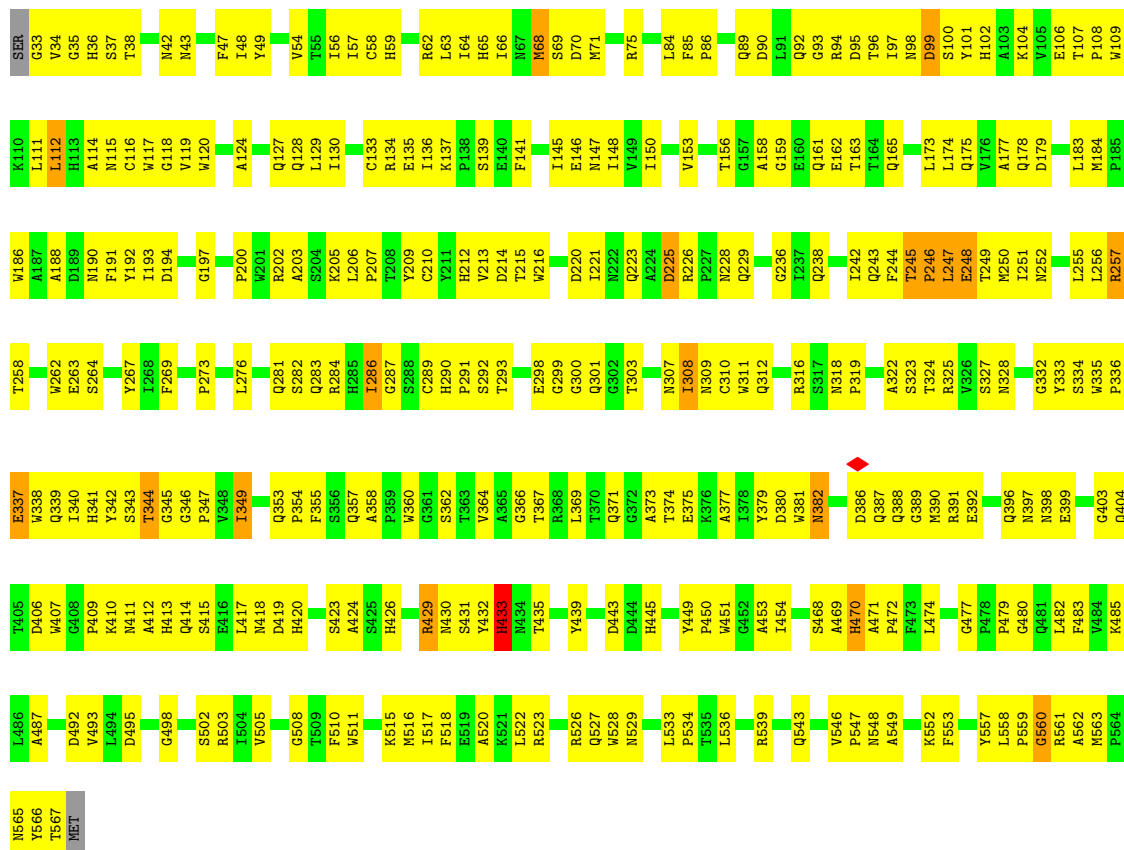
• Molecule 1: VP2

Chain U: 43% 53%





• Molecule 1: VP2



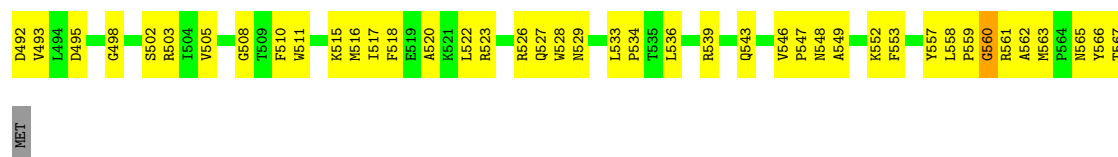
• Molecule 1: VP2

Opinion	Percentage
Doing a good job	43%
Doing a bad job	53%



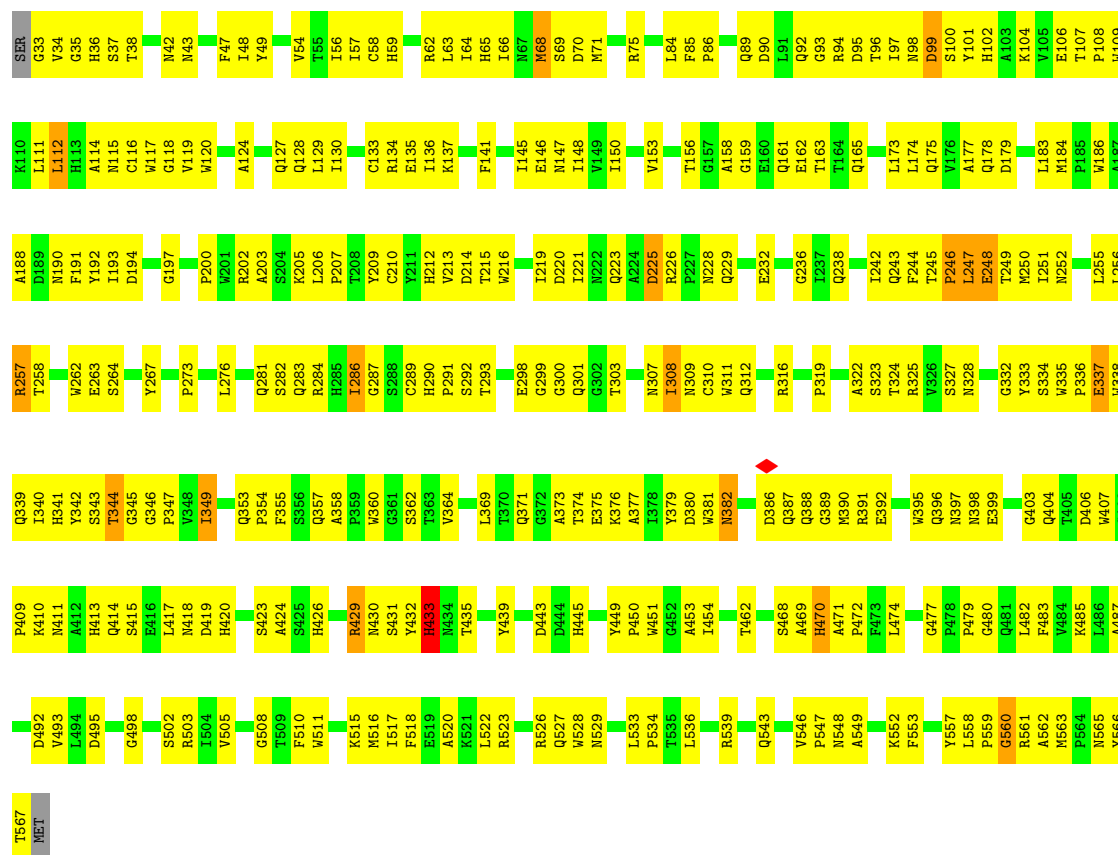
Opinion	Percentage
Doing a good job	43%
Doing a bad job	53%





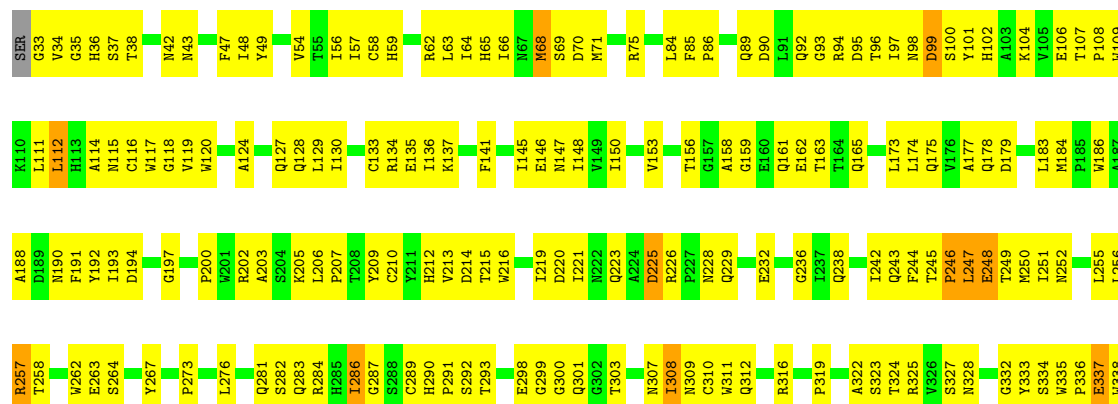
• Molecule 1: VP2

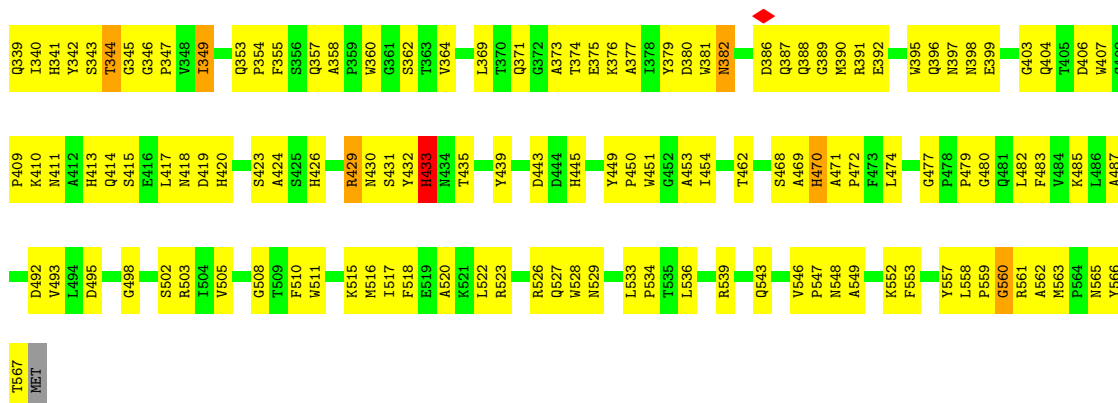
Chain Y: 43% 54% .



• Molecule 1: VP2

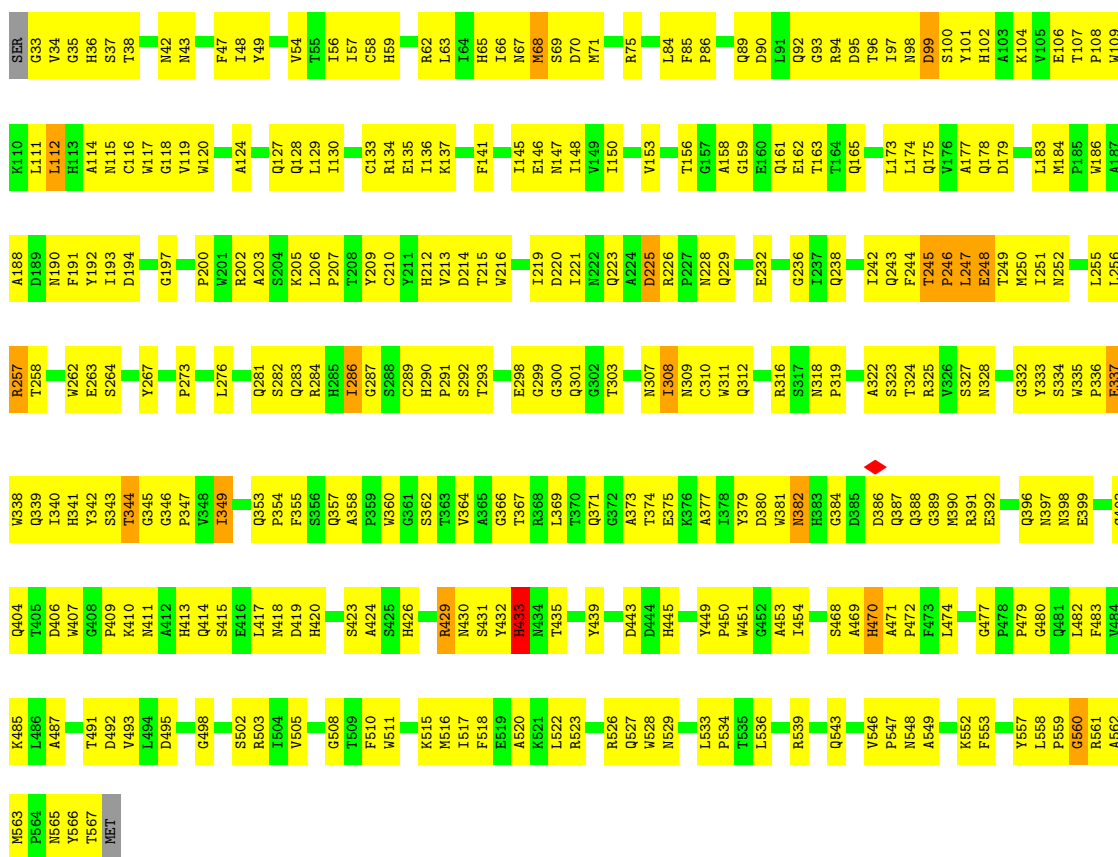
Chain Z: 43% 54% .





• Molecule 1: VP2

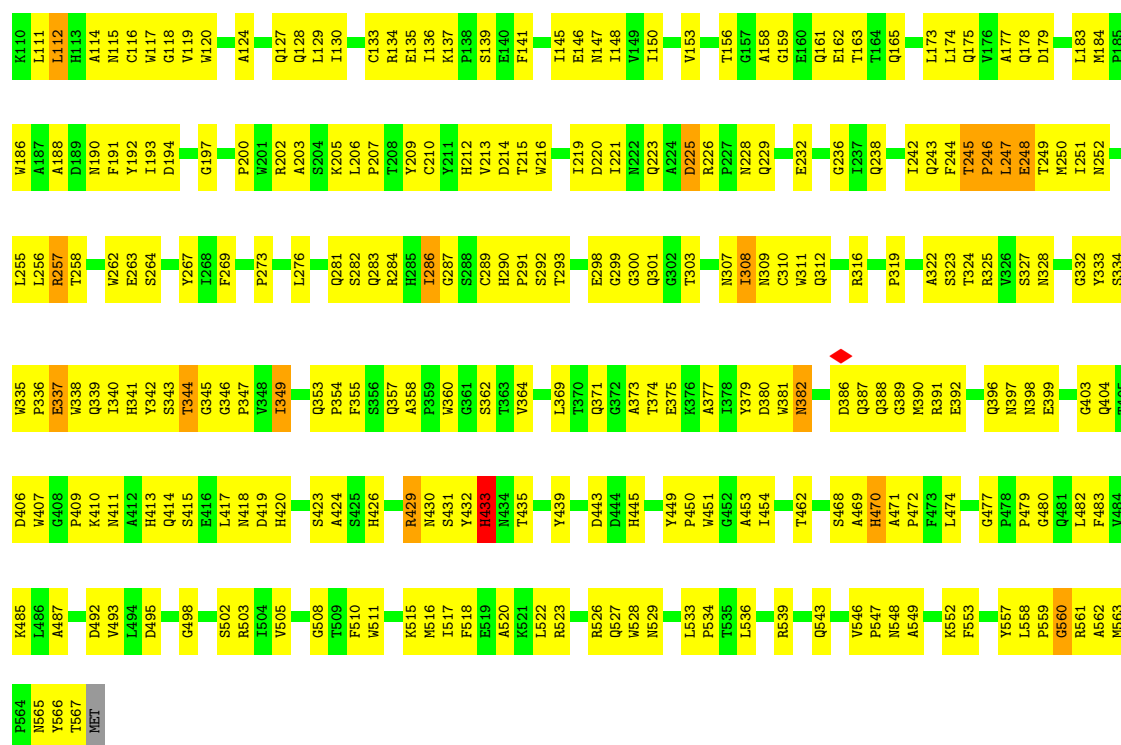
Chain 0: 42% 54%



• Molecule 1: VP2

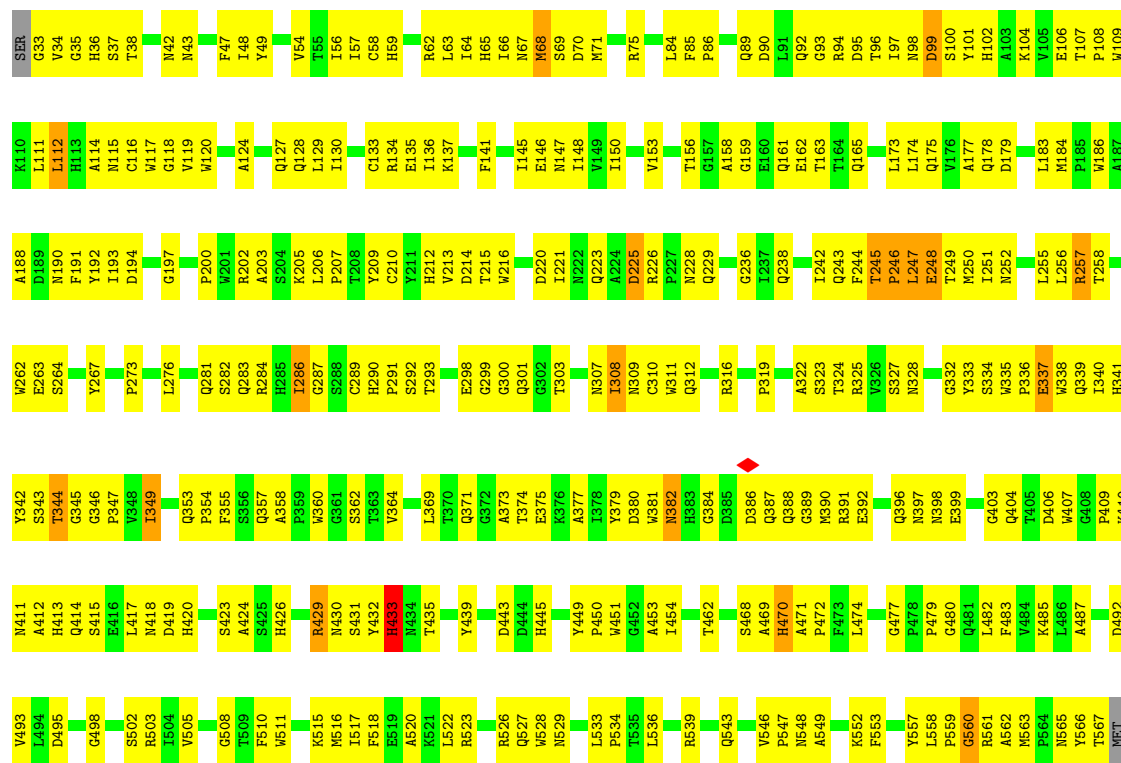
Chain 1: 43% 53%



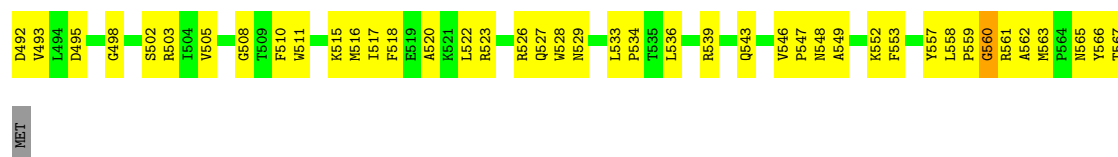


• Molecule 1: VP2

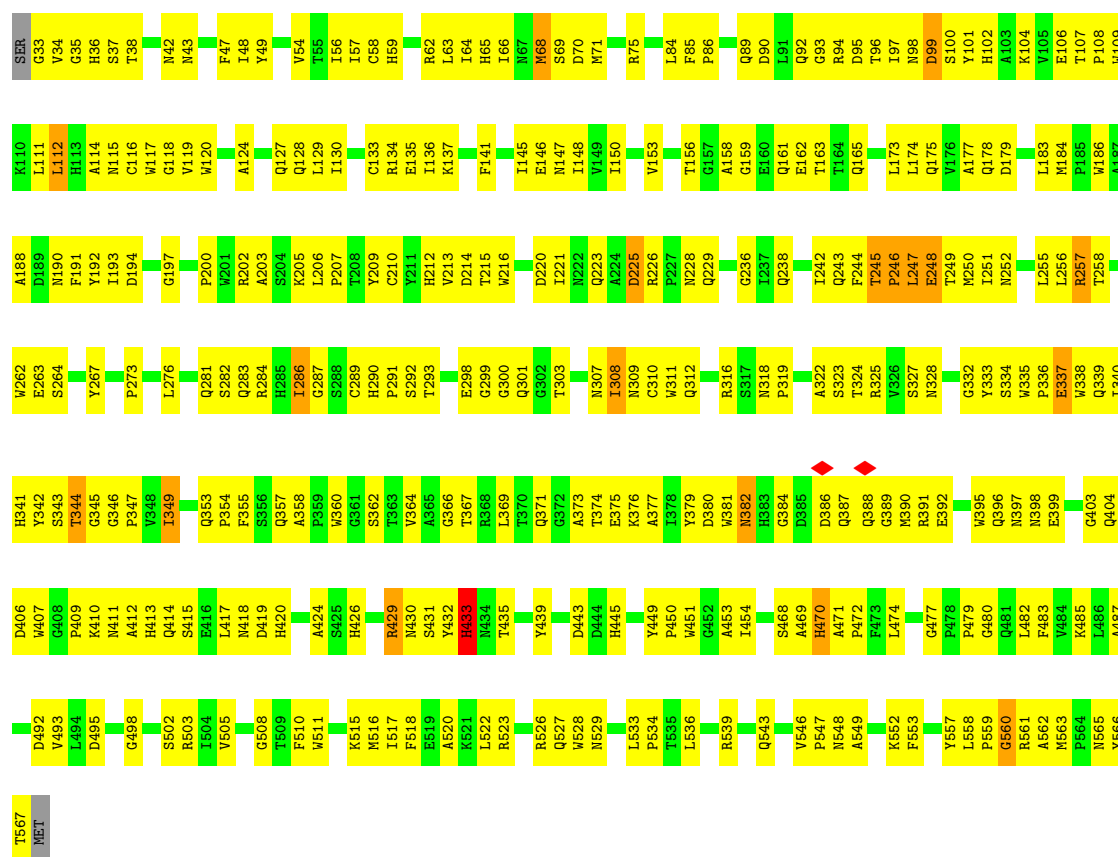
Chain 2: 43% 53% .



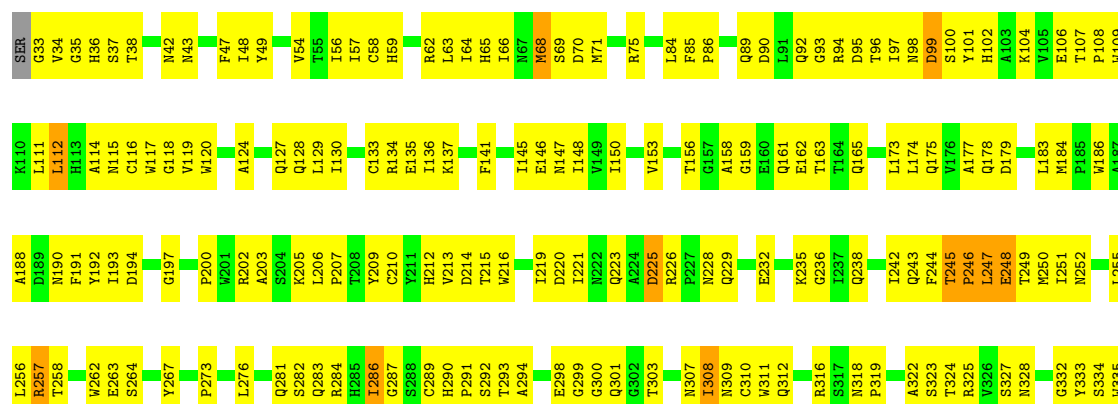
• Molecule 1: VP2

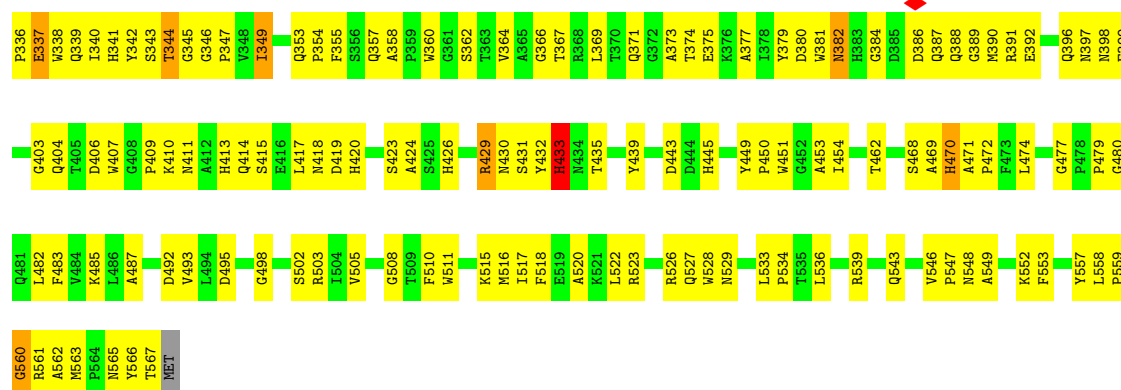


Molecule 1: VP2



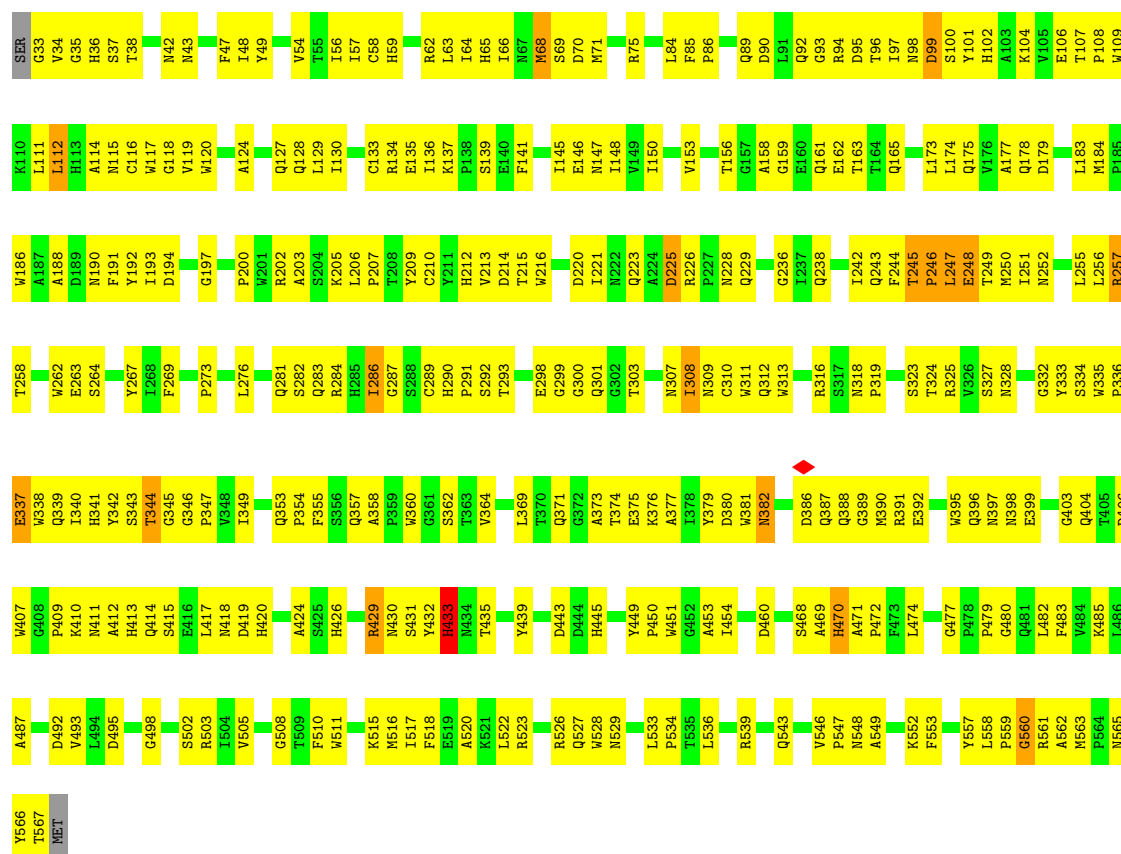
Molecule 1: VP2





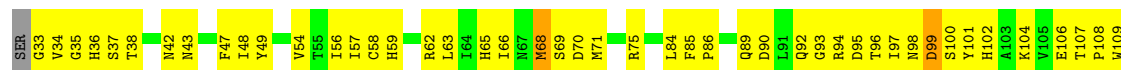
• Molecule 1: VP2

Chain b: 42% 54%



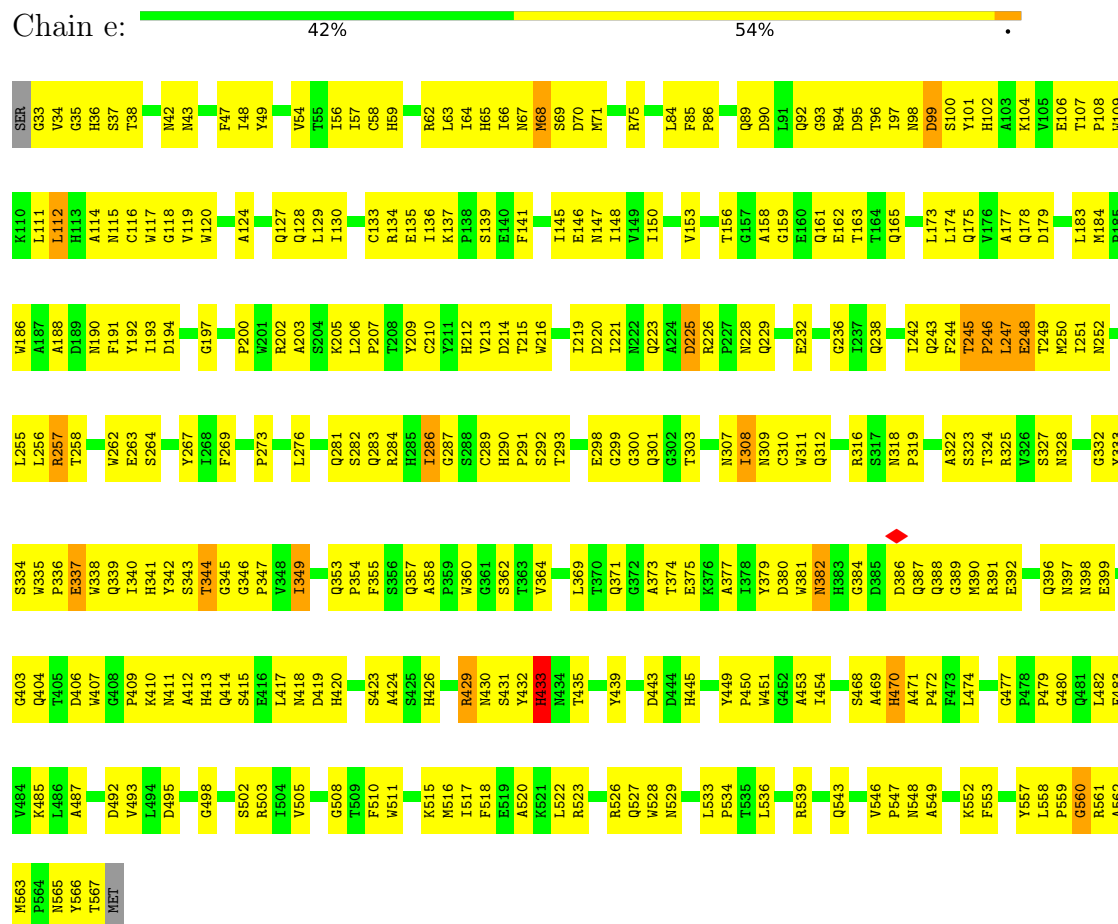
• Molecule 1: VP2

Chain c: 43% 53%

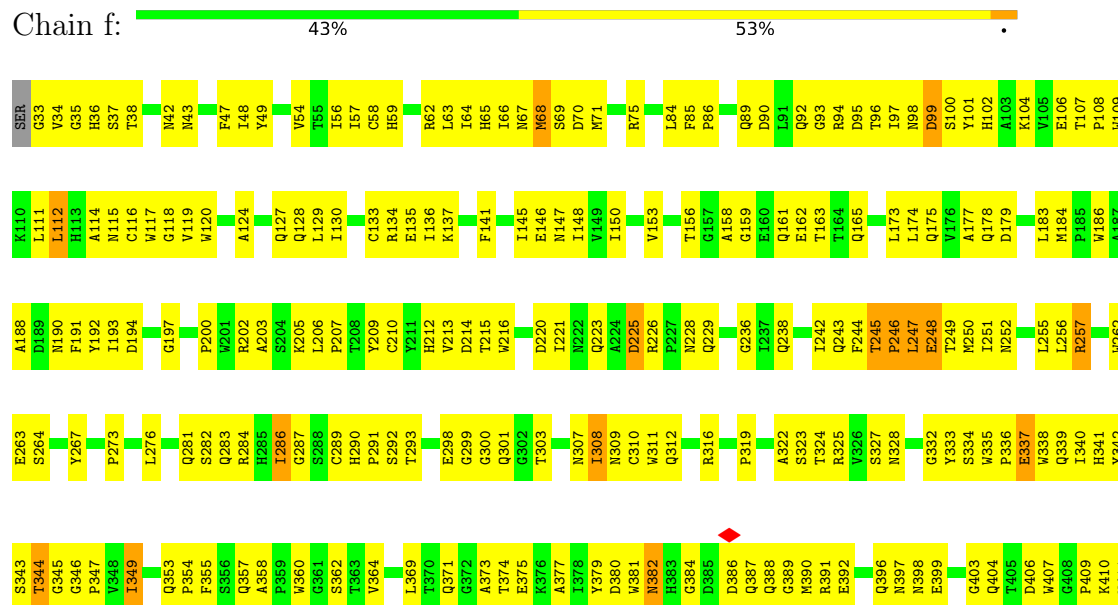


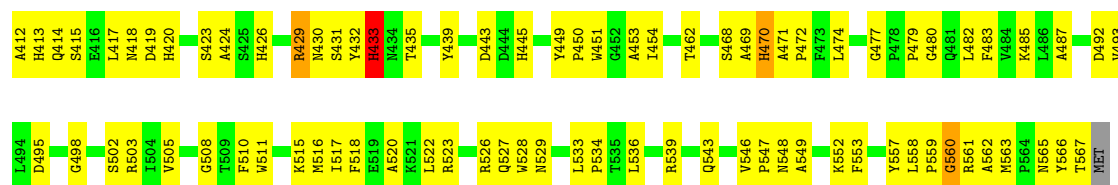
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• Molecule 1: VP2



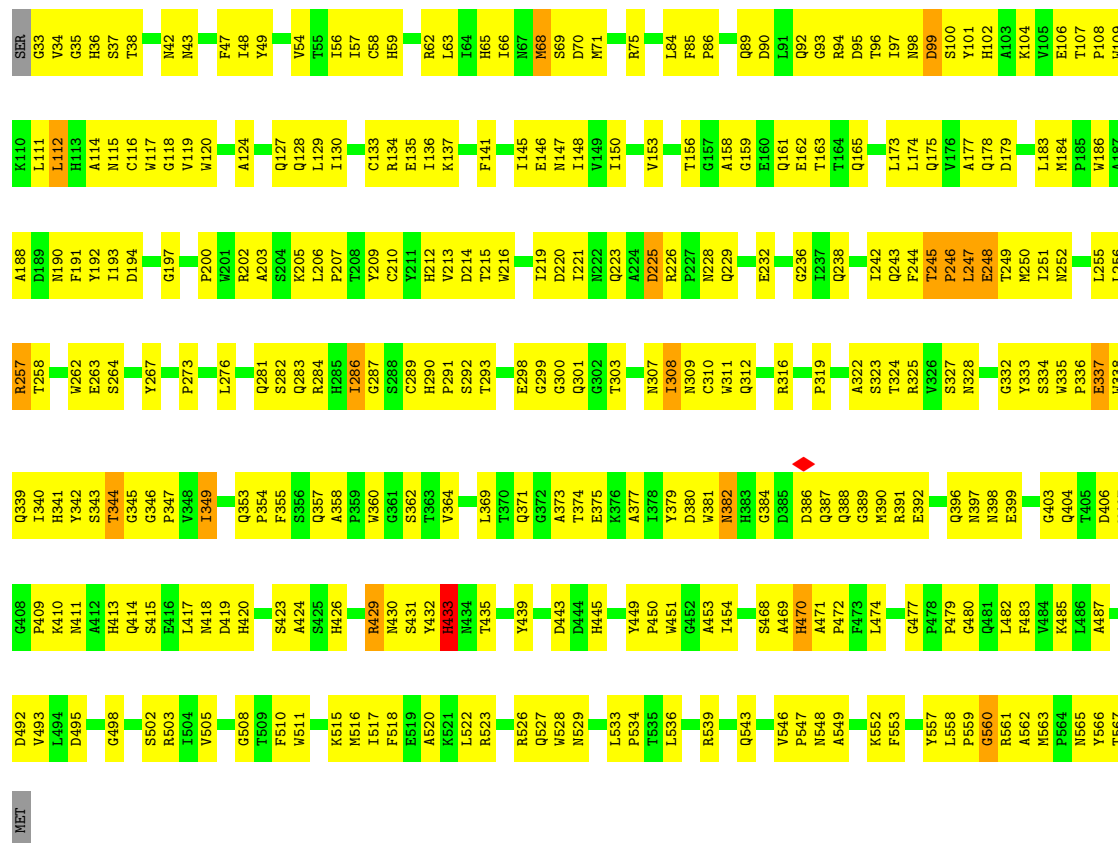
• Molecule 1: VP2





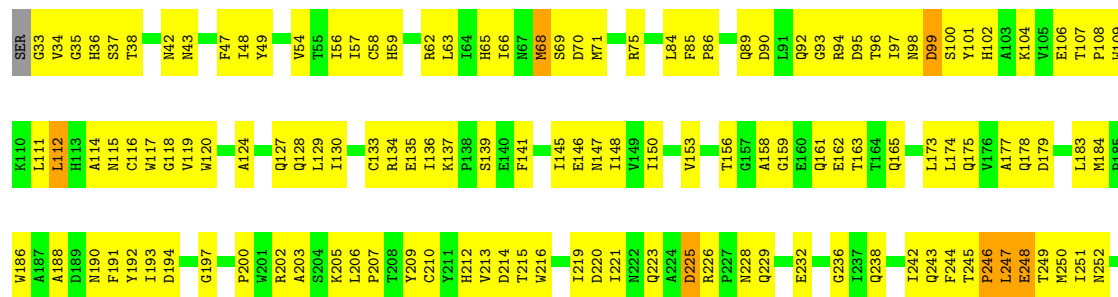
• Molecule 1: VP2

Chain g: 43% 53%



• Molecule 1: VP2

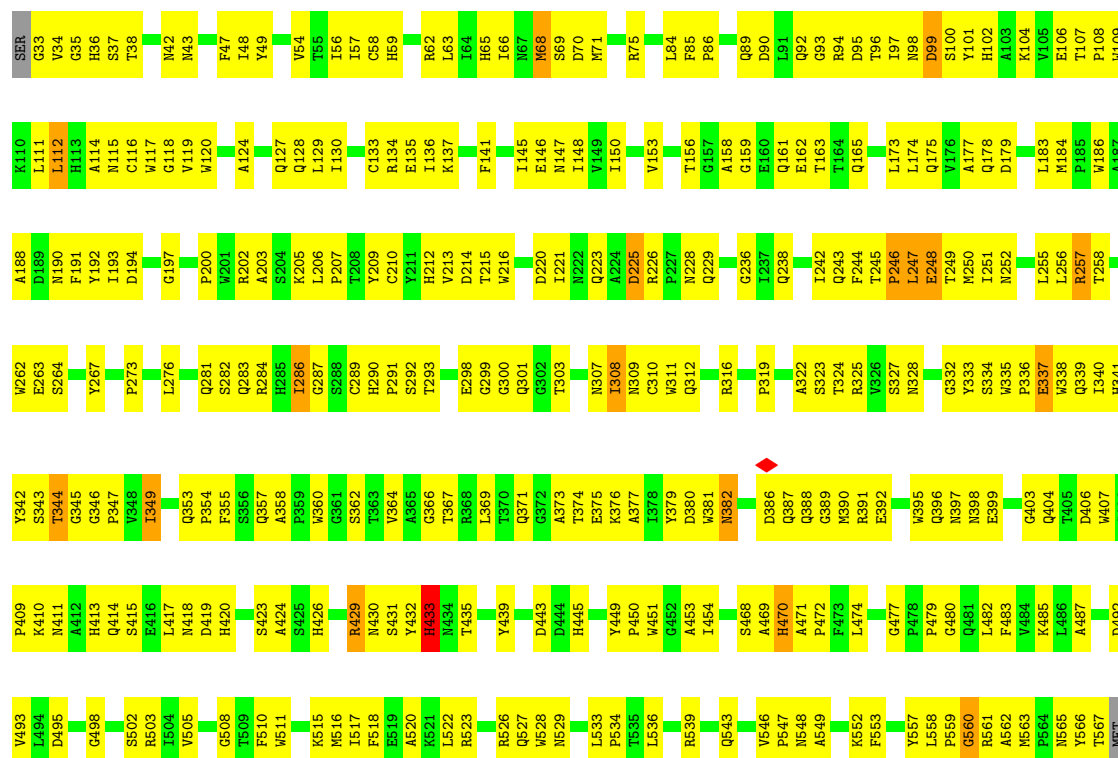
Chain h: 42% 54%





• Molecule 1: VP2

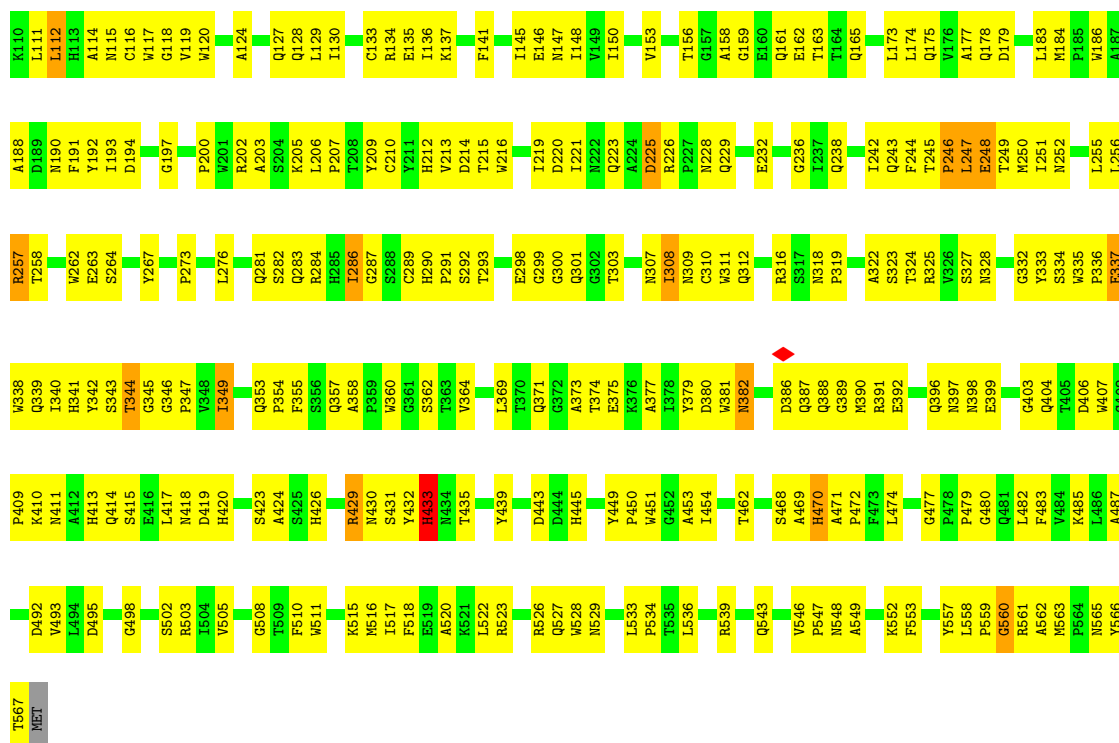
Chain i: 43% 53%



• Molecule 1: VP2

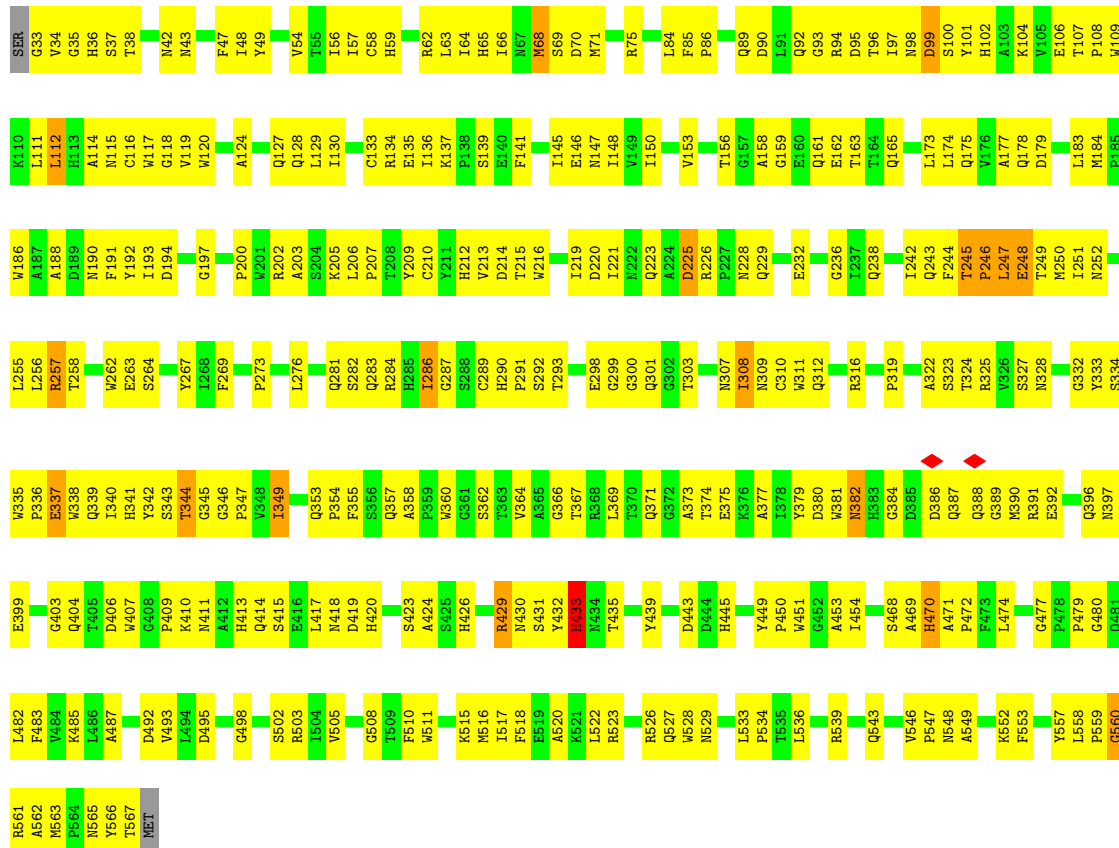
Chain j: 43% 54%



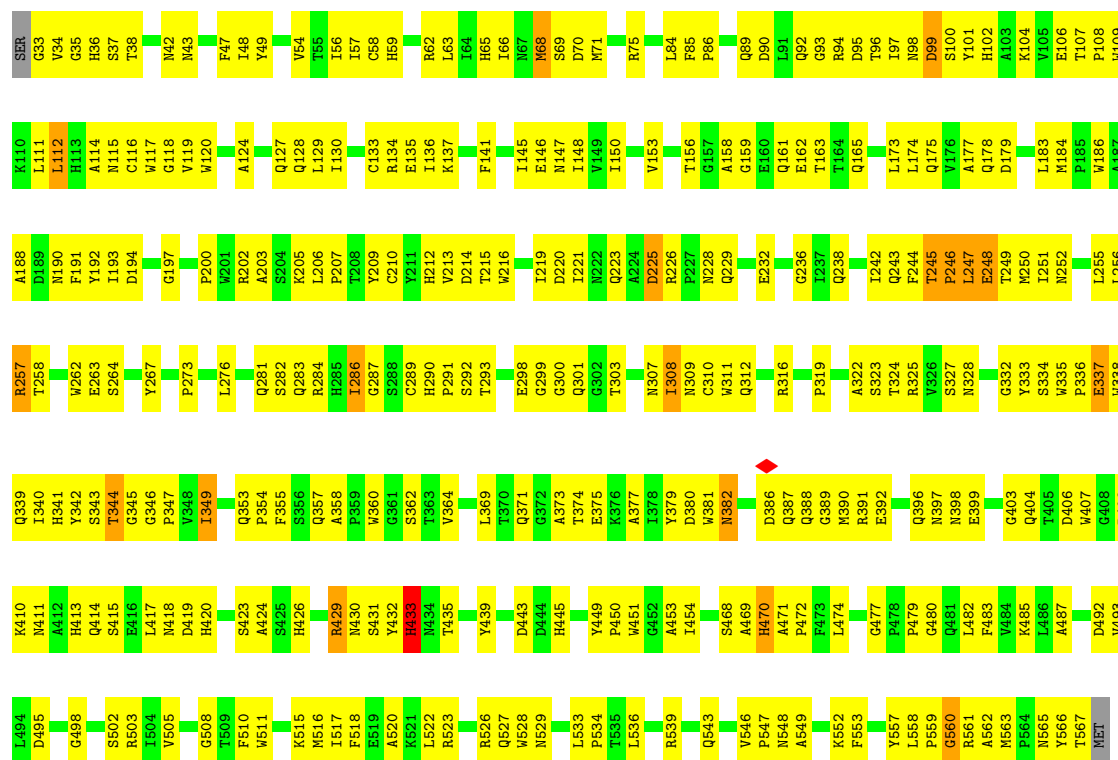


• Molecule 1: VP2

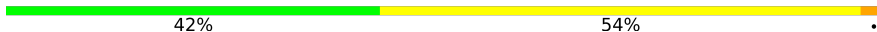
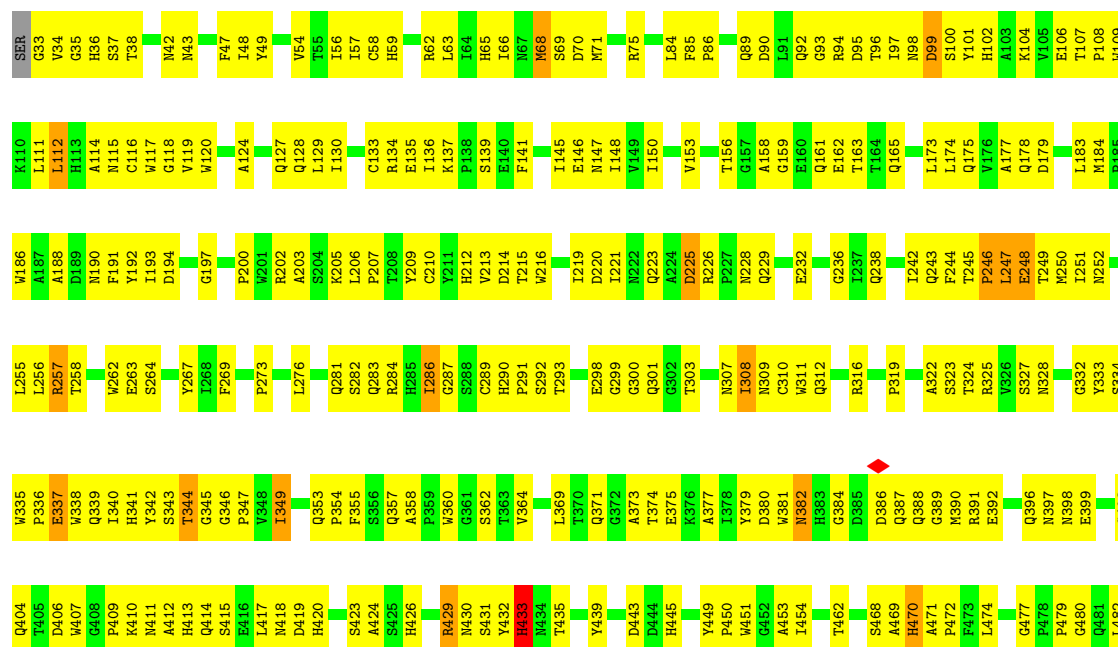
Chain k: 42% 54% .



● Molecule 1: VP2

Chain l:  43% 53%

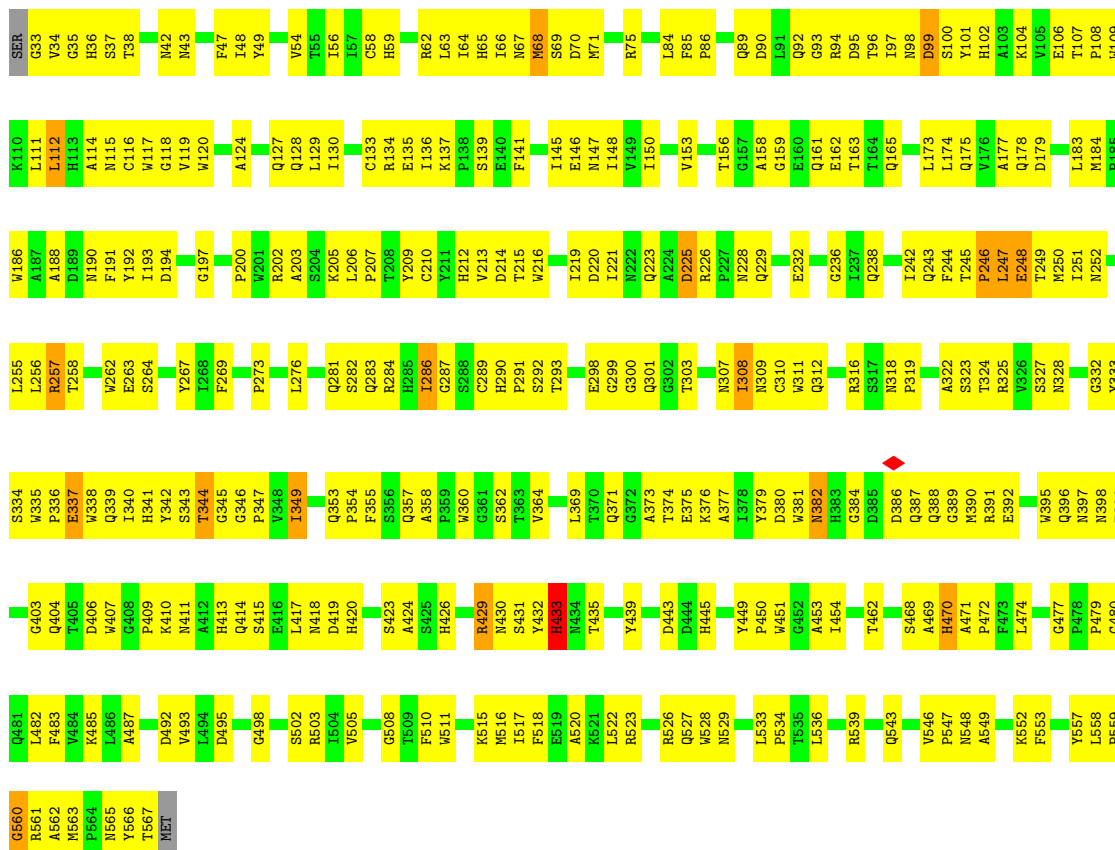
● Molecule 1: VP2

Chain m:  42% 54%



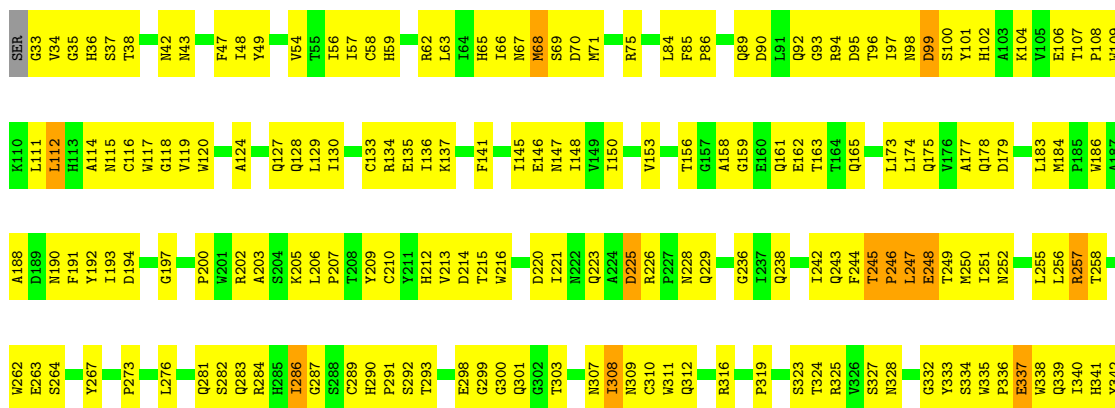
• Molecule 1: VP2

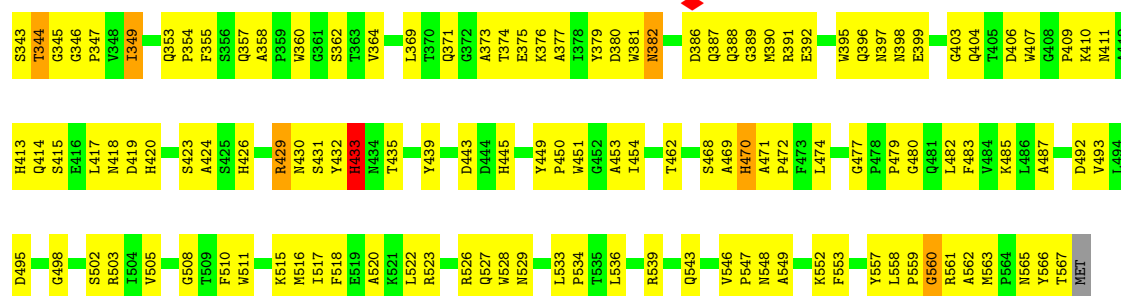
Chain n: 42% 54%



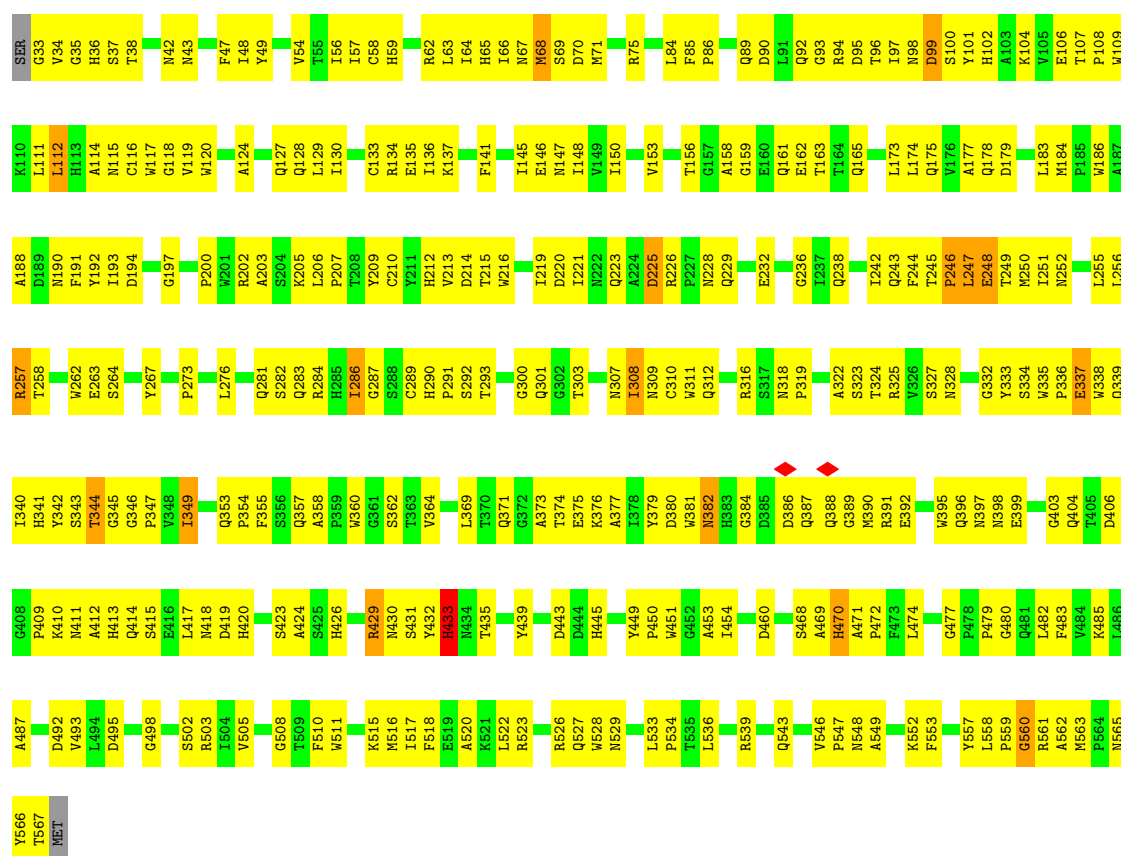
• Molecule 1: VP2

Chain o: 43% 53%

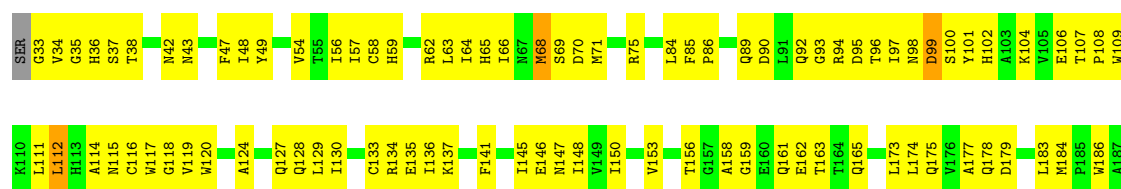


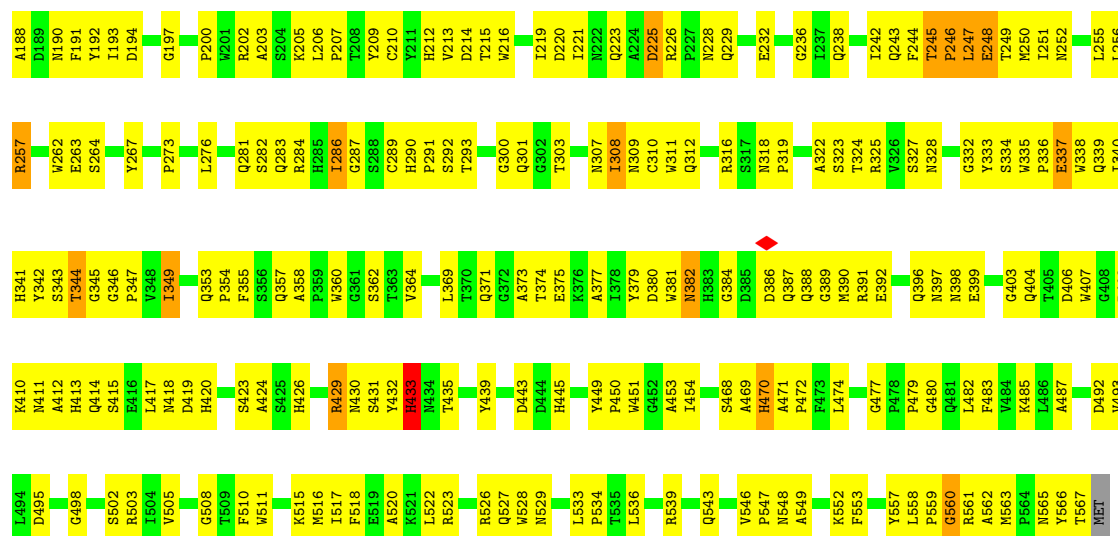


• Molecule 1: VP2

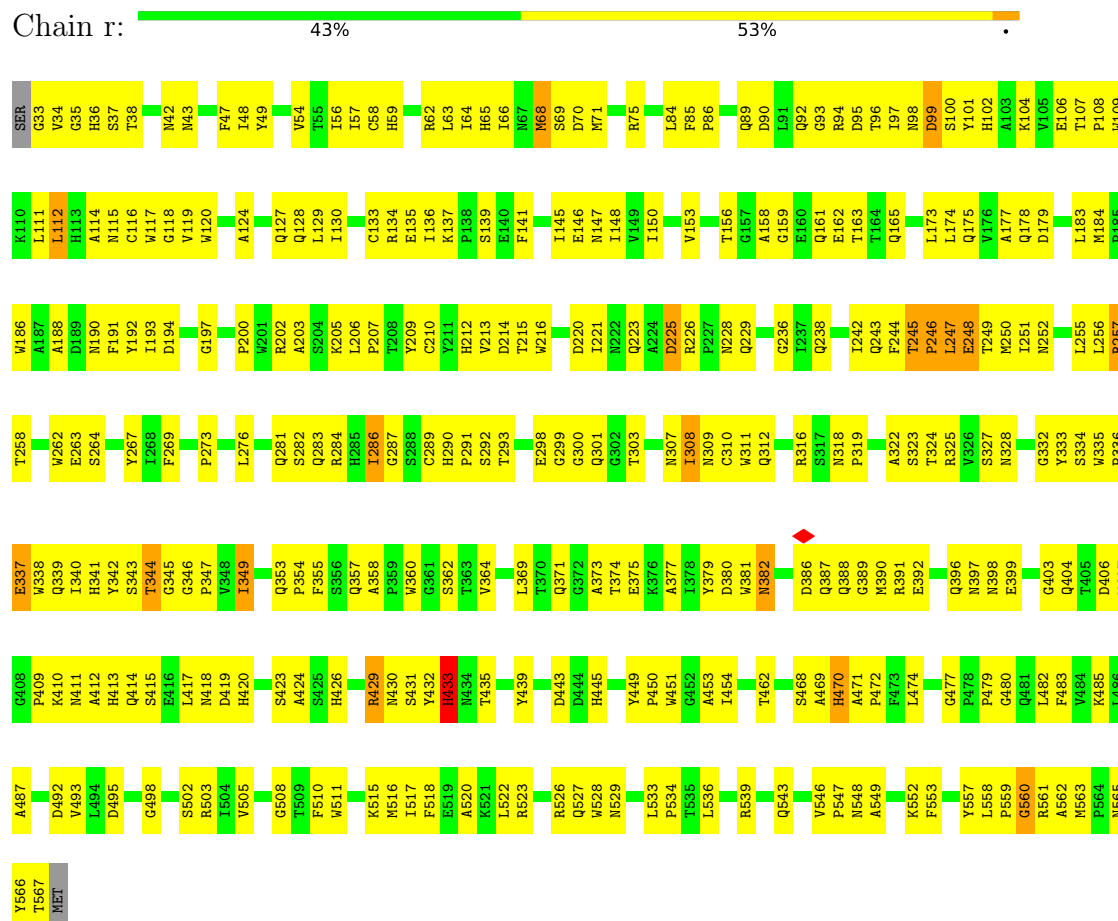


• Molecule 1: VP2





• Molecule 1: VP2

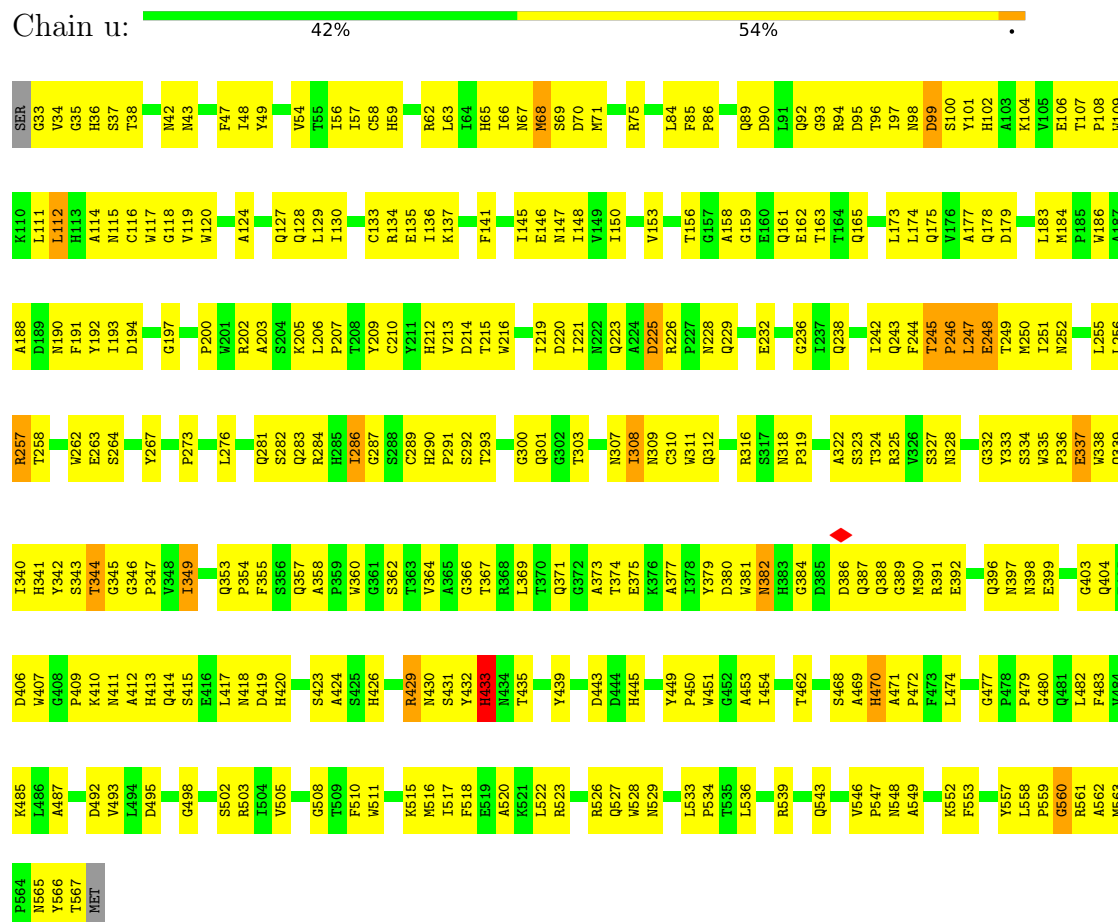


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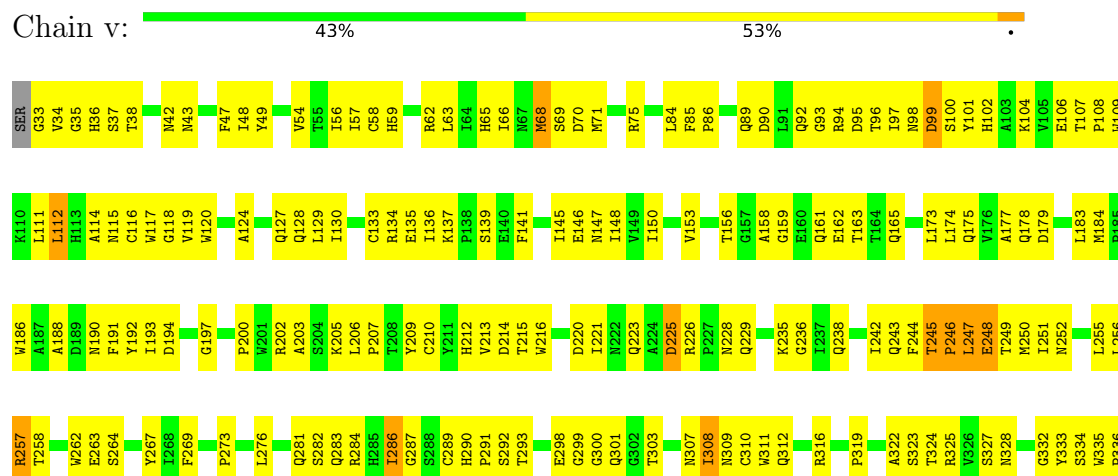


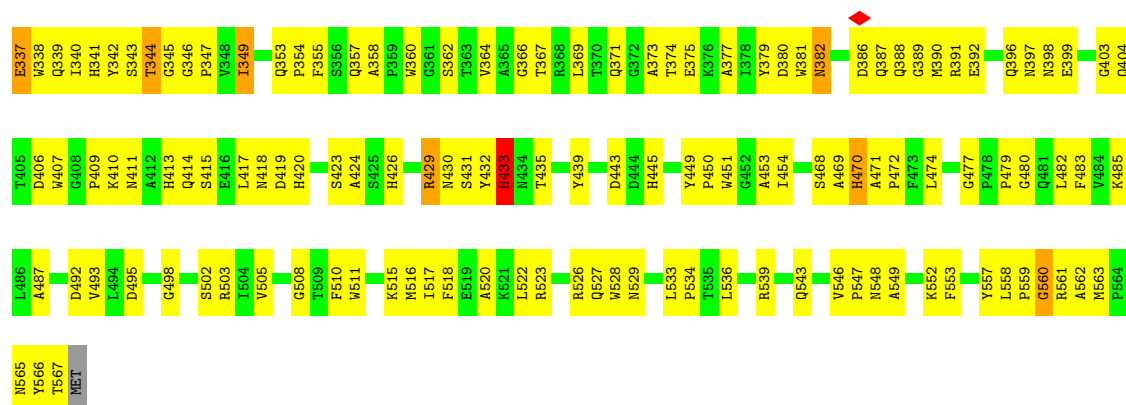


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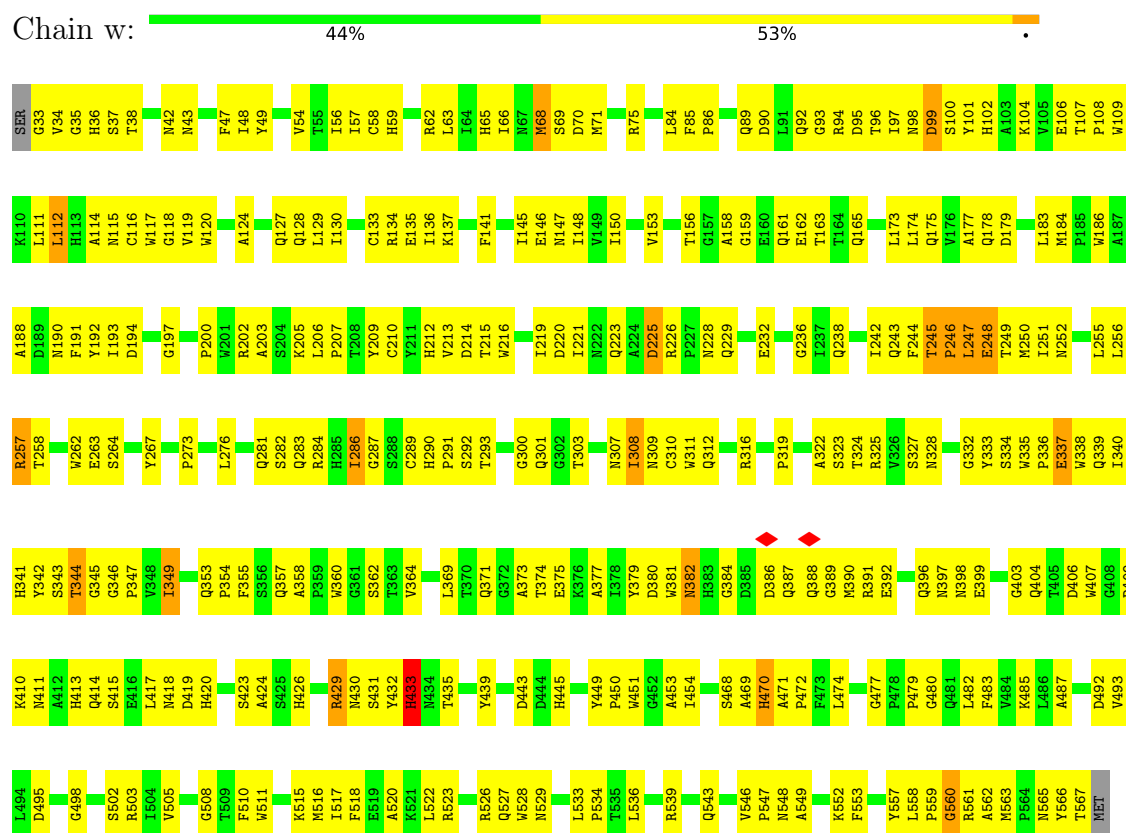


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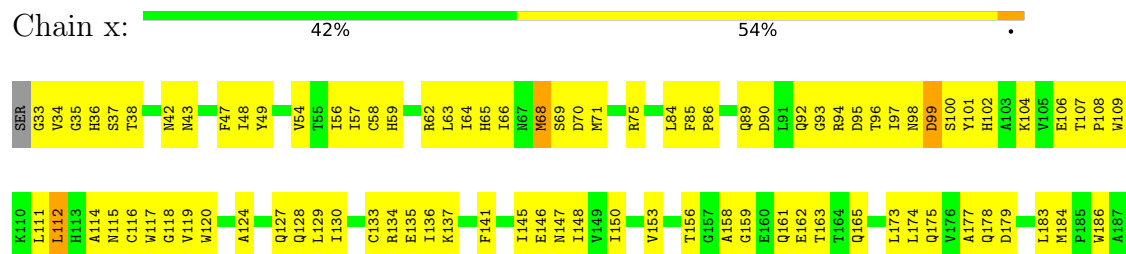


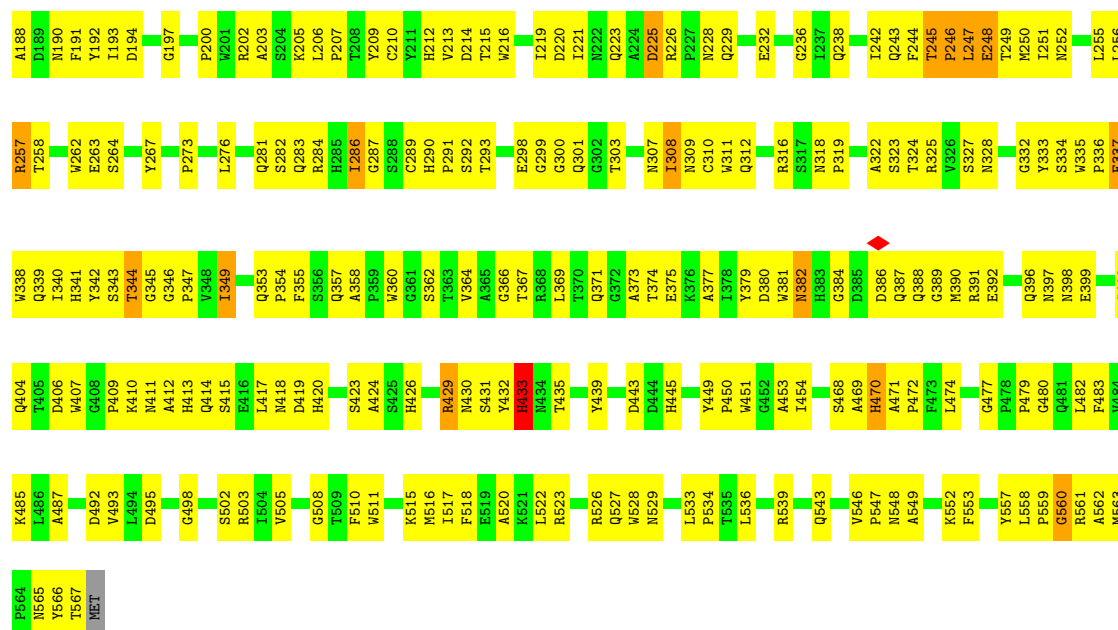


• Molecule 1: VP2



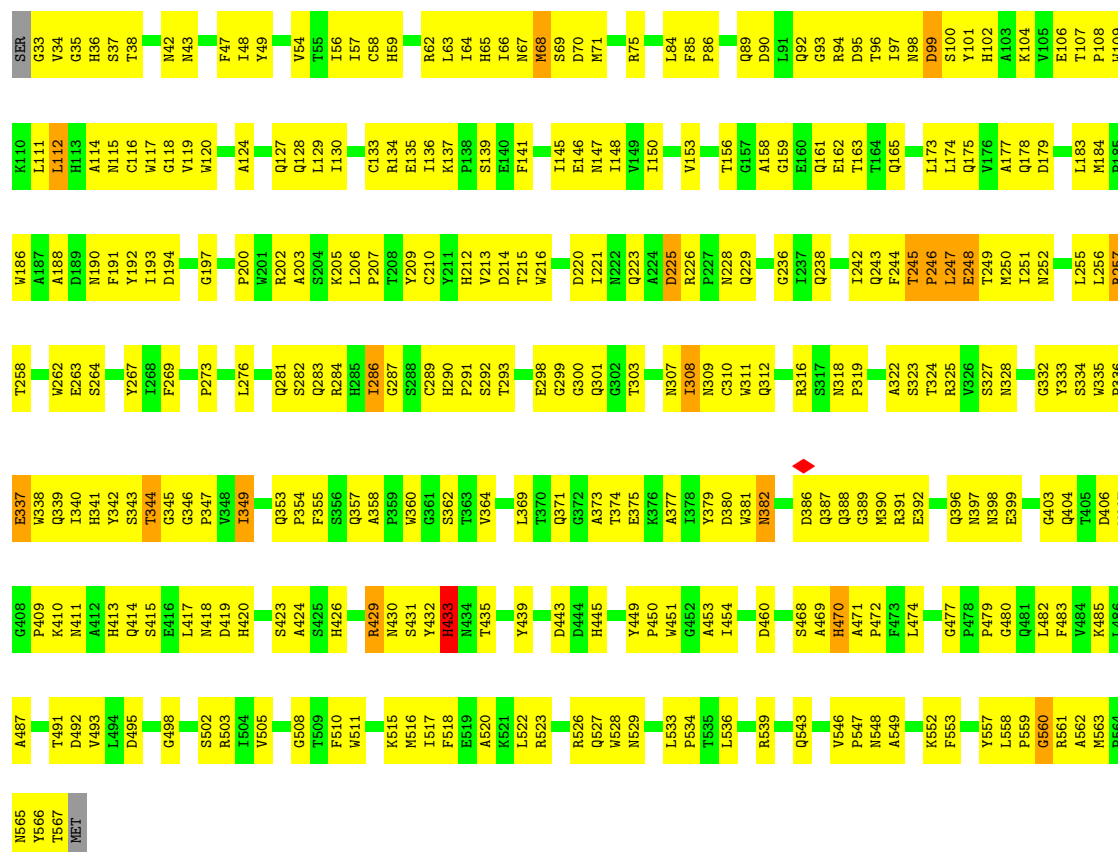
• Molecule 1: VP2



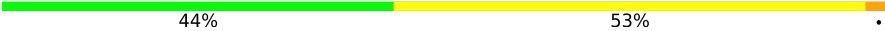


- Molecule 1: VP2

Chain y: 42% 54%



- Molecule 1: VP2

Chain z:  44% 53% .

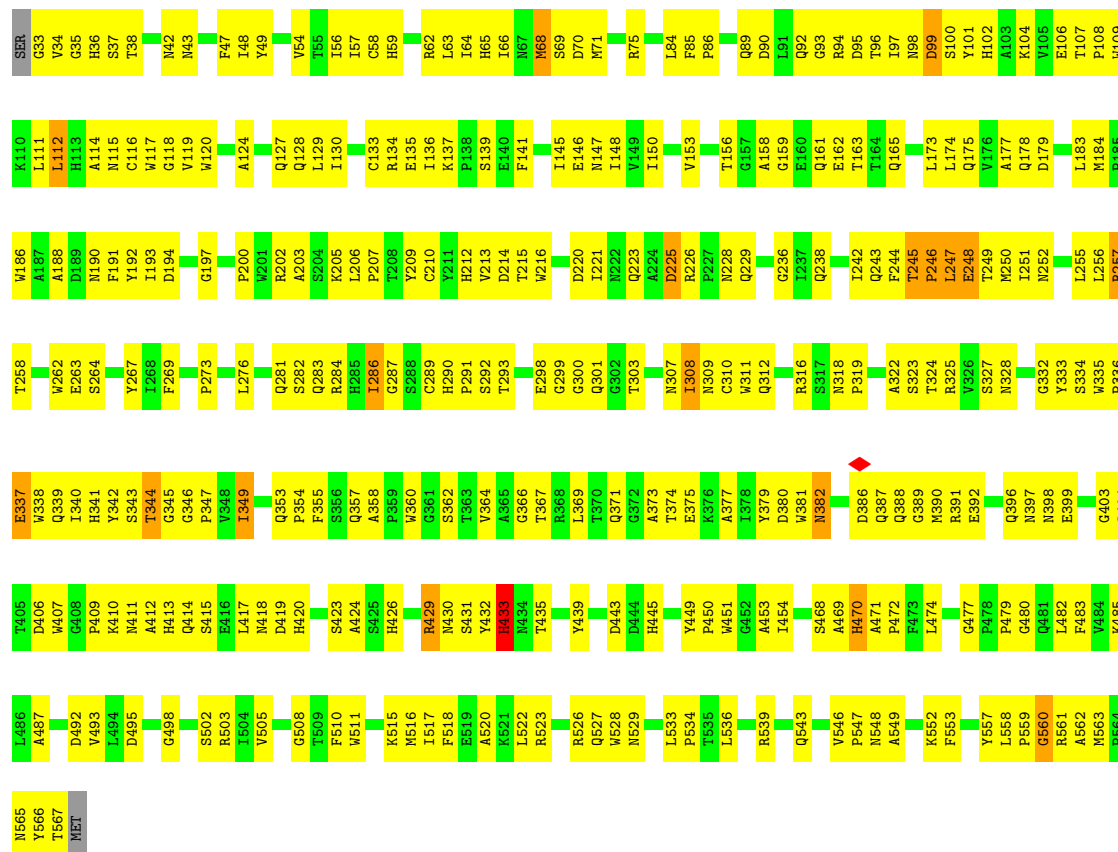
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H341	Y342	S343	T344	G346	P347	V348	I349	Q353	P354	F355	S356	Q357	A358	P359	W360	G361	S362	T363	V364	L369	T370	Q371	G372	A373	T374	E375	K376	A377	G378	Y379	D380	W381	N382	D386	Q387	Q388	G389	K390	R391	E392	Q396	N397	N398	E399	G403	Q404	T405	D406	G408	P409	K410	N411
R257	T258	W262	E263	S264	Y267	P273	L276	Q281	S282	Q283	R284	H285	T286	G287	S288	C289	H290	P291	V213	S292	T293	G300	Q301	G302	T303	N307	T308	N309	C310	W311	Q312	R316	P319	A322	S323	T324	R325	Q243	F244	T245	P246	E248	T249	N250	T251	N252	L255	L256				
A188	D189	N190	F191	Y192	G193	D194	G197	P200	W201	R202	A203	S204	K205	L206	P207	T208	Y209	C210	H212	V213	D214	T215	W216	G219	D220	I221	W222	Q223	A224	D225	R226	F227	N228	Q229	E232	G236	I237	Q238	L242	Q243	F244	T245	P246	E248	T249	N250	T251	N252	L255	L256		
K110	L111	L112	H113	A114	N115	C116	W117	G118	W119	W120	A124	Q127	Q128	L129	I130	C133	R134	E135	I136	K137	F141	I145	E146	N147	I148	V149	I150	V153	T156	G157	A158	G159	Q161	E162	T163	T164	Q165	L173	L174	Q175	V176	A177	Q178	D179	L183	M184	P185	W186	A187			
SER	G33	G34	G35	H36	S37	T38	N42	N43	F47	I48	Y49	V54	T55	I56	I57	C58	H59	R62	L63	T64	H65	I66	N67	M68	S69	D70	M71	R75	L84	F85	P86	Q89	D90	L91	Q92	G93	R94	D95	T96	I97	N98	D99	S100	Y101	H102	A103	K104	V105	E106	T107	P108	W109

• Molecule 1: VP2

Chain 6:  43% 53% .

V493	N411	T340	R257	A188	K110	SER
L494	A412	H341		D189	L111	
D495	H413	Y342	W262	N190	L112	G33
	Q414	S343	E263	F191	H113	V34
G498	S415	T344	S264	I192	A114	G35
	E416	G345		I193	N115	H36
S502	L417	G346	Y267	D194	C116	S37
R503	N418	P347			W117	T38
T504	D419	V348	P273	G197	G118	N42
V505	H420	I349			V119	N43
			L276	P200	W120	
G508	S423	Q353		W201		F47
T509	A424	P354	Q281	R202	A124	I48
F510	S425	P354	Q282	A203		Y49
W511	H426	S356	Q283	S204	Q127	
		Q357	H284	K205	Q128	V54
K515	R429	A358	R285	L206	L129	T55
M516	N430	P359	T286	P207	I130	I56
L517	L430	W360	G287	T208		I57
F518	Y432	G361	S288	Y209	C133	C58
E519	H433	S362	C289	C210	R134	H59
A520	N434	T363	H290	V211	E135	
K521	T435	V364	P291	H212	I136	R62
L522			S292	V213	K137	L63
R523	Y439	L369	T293	D214		T64
		T370	E298	T215	F141	H65
R526	D443	Q371	G299	W216		I66
Q527	D444	G372	G300		I145	N67
W528	H445	A373	Q301	T219	E146	M68
N529		T374	G302	D220	N147	S69
	Y449	E375	G303	I221	I148	D70
L533	P450	K376	T303	N222	V149	M71
P534	W451	A377		Q223	I150	
T535	G452	L378	N307	A224		R75
L536	A453	Y379	I308	D225	V153	
	I454	D380	N309	R226		L84
R539		W381	C310	F227	T156	F85
	D460	N382	W311	N228	G157	P86
			Q312	Q229	A158	
Q543					G159	Q89
V546	S468	D386	R316	E232	F160	D90
P547	A469	Q387			Q161	L91
N548	H470	Q388	P319	Q236	E162	Q92
A549	P472	G389		T237	T163	G93
	F473	K390	A322	Q238	T164	R94
K552	L474	R391	S323		Q165	D95
F553		E392	T324	T242		T96
			R325	Q243		I97
Y557	P478	Q396	V326	F244	L173	N98
L558	P479	N397	S327	T245	L174	
P559	Q480	N398	N328	P246	Q175	D99
G560	Q481	E399		L247	V176	S100
R561	L482		G332	E248	A177	Y101
A562	F483	G403	Y333	T249	Q178	H102
M563	V484	T405	S334	K250	D179	A103
P564	K485	T406	W335	I251	L183	K104
N565	L486	D406	P336	N252	M184	V105
Y566	A487	G407	E337		P185	E106
T567		G408	W338	L255	W186	P108
		P409	O220	T256	A187	W109

Chain 7: 42% 54% .



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	7564	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	57	Depositor
Minimum defocus (nm)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	Not provided	
Image detector	DIRECT ELECTRON DE-20 (5k x 3k)	Depositor
Maximum map value	17.508	Depositor
Minimum map value	-11.269	Depositor
Average map value	0.000	Depositor
Map value standard deviation	1.000	Depositor
Recommended contour level	1	Depositor
Map size (Å)	437.98, 437.98, 437.98	wwPDB
Map dimensions	359, 359, 359	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.22, 1.22, 1.22	Depositor

5 Model quality ⓘ

5.1 Standard geometry ⓘ

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
1	0	0.49	0/4472	0.79	14/6114 (0.2%)
1	1	0.49	0/4472	0.79	14/6114 (0.2%)
1	2	0.49	0/4472	0.79	14/6114 (0.2%)
1	3	0.49	0/4472	0.79	14/6114 (0.2%)
1	4	0.49	0/4472	0.79	14/6114 (0.2%)
1	5	0.49	0/4472	0.79	14/6114 (0.2%)
1	6	0.49	0/4472	0.79	14/6114 (0.2%)
1	7	0.49	0/4472	0.79	14/6114 (0.2%)
1	A	0.49	0/4472	0.79	14/6114 (0.2%)
1	B	0.49	0/4472	0.79	14/6114 (0.2%)
1	C	0.49	0/4472	0.79	14/6114 (0.2%)
1	D	0.49	0/4472	0.79	14/6114 (0.2%)
1	E	0.49	0/4472	0.79	14/6114 (0.2%)
1	F	0.49	0/4472	0.79	14/6114 (0.2%)
1	G	0.49	0/4472	0.79	14/6114 (0.2%)
1	H	0.49	0/4472	0.79	14/6114 (0.2%)
1	I	0.49	0/4472	0.79	14/6114 (0.2%)
1	J	0.49	0/4472	0.79	14/6114 (0.2%)
1	K	0.49	0/4472	0.79	14/6114 (0.2%)
1	L	0.49	0/4472	0.79	14/6114 (0.2%)
1	M	0.49	0/4472	0.79	14/6114 (0.2%)
1	N	0.49	0/4472	0.79	14/6114 (0.2%)
1	O	0.49	0/4472	0.79	14/6114 (0.2%)
1	P	0.49	0/4472	0.79	14/6114 (0.2%)
1	Q	0.49	0/4472	0.79	14/6114 (0.2%)
1	R	0.49	0/4472	0.79	14/6114 (0.2%)
1	S	0.49	0/4472	0.79	14/6114 (0.2%)
1	T	0.49	0/4472	0.79	14/6114 (0.2%)
1	U	0.49	0/4472	0.79	14/6114 (0.2%)
1	V	0.49	0/4472	0.79	14/6114 (0.2%)
1	W	0.49	0/4472	0.79	14/6114 (0.2%)
1	X	0.49	0/4472	0.79	14/6114 (0.2%)
1	Y	0.49	0/4472	0.79	14/6114 (0.2%)
1	Z	0.49	0/4472	0.79	14/6114 (0.2%)

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
1	a	0.49	0/4472	0.79	14/6114 (0.2%)
1	b	0.49	0/4472	0.79	14/6114 (0.2%)
1	c	0.49	0/4472	0.79	14/6114 (0.2%)
1	d	0.49	0/4472	0.79	14/6114 (0.2%)
1	e	0.49	0/4472	0.79	14/6114 (0.2%)
1	f	0.49	0/4472	0.79	14/6114 (0.2%)
1	g	0.49	0/4472	0.79	14/6114 (0.2%)
1	h	0.49	0/4472	0.79	14/6114 (0.2%)
1	i	0.49	0/4472	0.79	14/6114 (0.2%)
1	j	0.49	0/4472	0.79	14/6114 (0.2%)
1	k	0.49	0/4472	0.79	14/6114 (0.2%)
1	l	0.49	0/4472	0.79	14/6114 (0.2%)
1	m	0.49	0/4472	0.79	14/6114 (0.2%)
1	n	0.49	0/4472	0.79	14/6114 (0.2%)
1	o	0.49	0/4472	0.79	14/6114 (0.2%)
1	p	0.49	0/4472	0.79	14/6114 (0.2%)
1	q	0.49	0/4472	0.79	14/6114 (0.2%)
1	r	0.49	0/4472	0.79	14/6114 (0.2%)
1	s	0.49	0/4472	0.79	14/6114 (0.2%)
1	t	0.49	0/4472	0.79	14/6114 (0.2%)
1	u	0.49	0/4472	0.79	14/6114 (0.2%)
1	v	0.49	0/4472	0.79	14/6114 (0.2%)
1	w	0.49	0/4472	0.79	14/6114 (0.2%)
1	x	0.49	0/4472	0.79	14/6114 (0.2%)
1	y	0.49	0/4472	0.79	14/6114 (0.2%)
1	z	0.49	0/4472	0.79	14/6114 (0.2%)
All	All	0.49	0/268320	0.79	840/366840 (0.2%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	0	0	2
1	1	0	2
1	2	0	2
1	3	0	2
1	4	0	2
1	5	0	2
1	6	0	2
1	7	0	2

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Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	2
1	B	0	2
1	C	0	2
1	D	0	2
1	E	0	2
1	F	0	2
1	G	0	2
1	H	0	2
1	I	0	2
1	J	0	2
1	K	0	2
1	L	0	2
1	M	0	2
1	N	0	2
1	O	0	2
1	P	0	2
1	Q	0	2
1	R	0	2
1	S	0	2
1	T	0	2
1	U	0	2
1	V	0	2
1	W	0	2
1	X	0	2
1	Y	0	2
1	Z	0	2
1	a	0	2
1	b	0	2
1	c	0	2
1	d	0	2
1	e	0	2
1	f	0	2
1	g	0	2
1	h	0	2
1	i	0	2
1	j	0	2
1	k	0	2
1	l	0	2
1	m	0	2
1	n	0	2
1	o	0	2
1	p	0	2

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Mol	Chain	#Chirality outliers	#Planarity outliers
1	q	0	2
1	r	0	2
1	s	0	2
1	t	0	2
1	u	0	2
1	v	0	2
1	w	0	2
1	x	0	2
1	y	0	2
1	z	0	2
All	All	0	120

There are no bond length outliers.

The worst 5 of 840 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	r	245	THR	CA-C-N	10.94	131.38	119.90
1	r	245	THR	C-N-CA	10.94	131.38	119.90
1	7	245	THR	CA-C-N	10.94	131.38	119.90
1	7	245	THR	C-N-CA	10.94	131.38	119.90
1	E	245	THR	CA-C-N	10.93	131.37	119.90

There are no chirality outliers.

5 of 120 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	382	ASN	Peptide
1	A	68	MET	Peptide
1	B	382	ASN	Peptide
1	B	68	MET	Peptide
1	C	68	MET	Peptide

5.2 Too-close contacts [i](#)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	0	4326	0	4014	467	0
1	1	4326	0	4013	456	0
1	2	4326	0	4014	462	0
1	3	4326	0	4014	470	0
1	4	4326	0	4013	463	0
1	5	4326	0	4013	463	0
1	6	4326	0	4014	456	0
1	7	4326	0	4013	465	0
1	A	4326	0	4014	462	0
1	B	4326	0	4013	466	0
1	C	4326	0	4014	465	0
1	D	4326	0	4013	459	0
1	E	4326	0	4014	461	0
1	F	4326	0	4013	454	0
1	G	4326	0	4014	458	0
1	H	4326	0	4013	470	0
1	I	4326	0	4014	463	0
1	J	4326	0	4013	461	0
1	K	4326	0	4013	464	0
1	L	4326	0	4014	467	0
1	M	4326	0	4014	466	0
1	N	4326	0	4014	464	0
1	O	4326	0	4014	466	0
1	P	4326	0	4013	463	0
1	Q	4326	0	4014	464	0
1	R	4326	0	4014	461	0
1	S	4326	0	4013	454	0
1	T	4326	0	4014	462	0
1	U	4326	0	4014	461	0
1	V	4326	0	4014	469	0
1	W	4326	0	4014	468	0
1	X	4326	0	4013	463	0
1	Y	4326	0	4014	464	0
1	Z	4326	0	4014	464	0
1	a	4326	0	4013	463	0
1	b	4326	0	4014	470	0
1	c	4326	0	4013	456	0
1	d	4326	0	4013	465	0
1	e	4326	0	4014	469	0
1	f	4326	0	4014	459	0
1	g	4326	0	4014	462	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	h	4326	0	4014	466	0
1	i	4326	0	4014	461	0
1	j	4326	0	4014	466	0
1	k	4326	0	4014	465	0
1	l	4326	0	4014	461	0
1	m	4326	0	4014	465	0
1	n	4326	0	4014	465	0
1	o	4326	0	4013	456	0
1	p	4326	0	4014	462	0
1	q	4326	0	4014	459	0
1	r	4326	0	4014	463	0
1	s	4326	0	4013	465	0
1	t	4326	0	4014	464	0
1	u	4326	0	4014	461	0
1	v	4326	0	4014	458	0
1	w	4326	0	4014	463	0
1	x	4326	0	4013	467	0
1	y	4326	0	4014	460	0
1	z	4326	0	4013	450	0
All	All	259560	0	240820	21372	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 43.

The worst 5 of 21372 close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:X:34:VAL:N	1:5:36:HIS:CE1	1.71	1.58
1:a:34:VAL:N	1:e:36:HIS:CE1	1.71	1.58
1:J:36:HIS:CE1	1:0:34:VAL:N	1.72	1.58
1:p:34:VAL:H	1:u:36:HIS:CE1	1.22	1.58
1:h:34:VAL:H	1:l:36:HIS:CE1	1.22	1.58

There are no symmetry-related clashes.

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all PDB entries followed by that with respect to all EM entries.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	0	533/537 (99%)	508 (95%)	24 (4%)	1 (0%)	43	73
1	1	533/537 (99%)	508 (95%)	24 (4%)	1 (0%)	43	73
1	2	533/537 (99%)	508 (95%)	24 (4%)	1 (0%)	43	73
1	3	533/537 (99%)	508 (95%)	24 (4%)	1 (0%)	43	73
1	4	533/537 (99%)	508 (95%)	24 (4%)	1 (0%)	43	73
1	5	533/537 (99%)	508 (95%)	24 (4%)	1 (0%)	43	73
1	6	533/537 (99%)	508 (95%)	24 (4%)	1 (0%)	43	73
1	7	533/537 (99%)	508 (95%)	24 (4%)	1 (0%)	43	73
1	A	533/537 (99%)	508 (95%)	24 (4%)	1 (0%)	43	73
1	B	533/537 (99%)	508 (95%)	24 (4%)	1 (0%)	43	73
1	C	533/537 (99%)	508 (95%)	24 (4%)	1 (0%)	43	73
1	D	533/537 (99%)	508 (95%)	24 (4%)	1 (0%)	43	73
1	E	533/537 (99%)	508 (95%)	24 (4%)	1 (0%)	43	73
1	F	533/537 (99%)	508 (95%)	24 (4%)	1 (0%)	43	73
1	G	533/537 (99%)	508 (95%)	24 (4%)	1 (0%)	43	73
1	H	533/537 (99%)	508 (95%)	24 (4%)	1 (0%)	43	73
1	I	533/537 (99%)	508 (95%)	24 (4%)	1 (0%)	43	73
1	J	533/537 (99%)	508 (95%)	24 (4%)	1 (0%)	43	73
1	K	533/537 (99%)	508 (95%)	24 (4%)	1 (0%)	43	73
1	L	533/537 (99%)	508 (95%)	24 (4%)	1 (0%)	43	73
1	M	533/537 (99%)	508 (95%)	24 (4%)	1 (0%)	43	73
1	N	533/537 (99%)	508 (95%)	24 (4%)	1 (0%)	43	73
1	O	533/537 (99%)	508 (95%)	24 (4%)	1 (0%)	43	73
1	P	533/537 (99%)	508 (95%)	24 (4%)	1 (0%)	43	73
1	Q	533/537 (99%)	508 (95%)	24 (4%)	1 (0%)	43	73

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	R	533/537 (99%)	508 (95%)	24 (4%)	1 (0%)	43	73
1	S	533/537 (99%)	508 (95%)	24 (4%)	1 (0%)	43	73
1	T	533/537 (99%)	508 (95%)	24 (4%)	1 (0%)	43	73
1	U	533/537 (99%)	508 (95%)	24 (4%)	1 (0%)	43	73
1	V	533/537 (99%)	508 (95%)	24 (4%)	1 (0%)	43	73
1	W	533/537 (99%)	508 (95%)	24 (4%)	1 (0%)	43	73
1	X	533/537 (99%)	508 (95%)	24 (4%)	1 (0%)	43	73
1	Y	533/537 (99%)	508 (95%)	24 (4%)	1 (0%)	43	73
1	Z	533/537 (99%)	507 (95%)	25 (5%)	1 (0%)	43	73
1	a	533/537 (99%)	508 (95%)	24 (4%)	1 (0%)	43	73
1	b	533/537 (99%)	508 (95%)	24 (4%)	1 (0%)	43	73
1	c	533/537 (99%)	508 (95%)	24 (4%)	1 (0%)	43	73
1	d	533/537 (99%)	508 (95%)	24 (4%)	1 (0%)	43	73
1	e	533/537 (99%)	508 (95%)	24 (4%)	1 (0%)	43	73
1	f	533/537 (99%)	508 (95%)	24 (4%)	1 (0%)	43	73
1	g	533/537 (99%)	508 (95%)	24 (4%)	1 (0%)	43	73
1	h	533/537 (99%)	508 (95%)	24 (4%)	1 (0%)	43	73
1	i	533/537 (99%)	508 (95%)	24 (4%)	1 (0%)	43	73
1	j	533/537 (99%)	508 (95%)	24 (4%)	1 (0%)	43	73
1	k	533/537 (99%)	508 (95%)	24 (4%)	1 (0%)	43	73
1	l	533/537 (99%)	508 (95%)	24 (4%)	1 (0%)	43	73
1	m	533/537 (99%)	508 (95%)	24 (4%)	1 (0%)	43	73
1	n	533/537 (99%)	508 (95%)	24 (4%)	1 (0%)	43	73
1	o	533/537 (99%)	508 (95%)	24 (4%)	1 (0%)	43	73
1	p	533/537 (99%)	508 (95%)	24 (4%)	1 (0%)	43	73
1	q	533/537 (99%)	508 (95%)	24 (4%)	1 (0%)	43	73
1	r	533/537 (99%)	508 (95%)	24 (4%)	1 (0%)	43	73
1	s	533/537 (99%)	508 (95%)	24 (4%)	1 (0%)	43	73
1	t	533/537 (99%)	508 (95%)	24 (4%)	1 (0%)	43	73
1	u	533/537 (99%)	508 (95%)	24 (4%)	1 (0%)	43	73
1	v	533/537 (99%)	508 (95%)	24 (4%)	1 (0%)	43	73

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	w	533/537 (99%)	508 (95%)	24 (4%)	1 (0%)	43	73
1	x	533/537 (99%)	508 (95%)	24 (4%)	1 (0%)	43	73
1	y	533/537 (99%)	508 (95%)	24 (4%)	1 (0%)	43	73
1	z	533/537 (99%)	508 (95%)	24 (4%)	1 (0%)	43	73
All	All	31980/32220 (99%)	30479 (95%)	1441 (4%)	60 (0%)	44	73

5 of 60 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	193	ILE
1	H	193	ILE
1	S	193	ILE
1	V	193	ILE
1	1	193	ILE

5.3.2 Protein sidechains ⓘ

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all PDB entries followed by that with respect to all EM entries.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	0	464/466 (100%)	452 (97%)	12 (3%)	40	60
1	1	464/466 (100%)	452 (97%)	12 (3%)	40	60
1	2	464/466 (100%)	452 (97%)	12 (3%)	40	60
1	3	464/466 (100%)	452 (97%)	12 (3%)	40	60
1	4	464/466 (100%)	452 (97%)	12 (3%)	40	60
1	5	464/466 (100%)	452 (97%)	12 (3%)	40	60
1	6	464/466 (100%)	452 (97%)	12 (3%)	40	60
1	7	464/466 (100%)	452 (97%)	12 (3%)	40	60
1	A	464/466 (100%)	452 (97%)	12 (3%)	40	60
1	B	464/466 (100%)	452 (97%)	12 (3%)	40	60
1	C	464/466 (100%)	452 (97%)	12 (3%)	40	60
1	D	464/466 (100%)	452 (97%)	12 (3%)	40	60

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles		
1	E	464/466 (100%)	452 (97%)	12 (3%)	40	60	
1	F	464/466 (100%)	452 (97%)	12 (3%)	40	60	
1	G	464/466 (100%)	452 (97%)	12 (3%)	40	60	
1	H	464/466 (100%)	452 (97%)	12 (3%)	40	60	
1	I	464/466 (100%)	452 (97%)	12 (3%)	40	60	
1	J	464/466 (100%)	452 (97%)	12 (3%)	40	60	
1	K	464/466 (100%)	452 (97%)	12 (3%)	40	60	
1	L	464/466 (100%)	452 (97%)	12 (3%)	40	60	
1	M	464/466 (100%)	452 (97%)	12 (3%)	40	60	
1	N	464/466 (100%)	452 (97%)	12 (3%)	40	60	
1	O	464/466 (100%)	452 (97%)	12 (3%)	40	60	
1	P	464/466 (100%)	452 (97%)	12 (3%)	40	60	
1	Q	464/466 (100%)	452 (97%)	12 (3%)	40	60	
1	R	464/466 (100%)	452 (97%)	12 (3%)	40	60	
1	S	464/466 (100%)	452 (97%)	12 (3%)	40	60	
1	T	464/466 (100%)	452 (97%)	12 (3%)	40	60	
1	U	464/466 (100%)	452 (97%)	12 (3%)	40	60	
1	V	464/466 (100%)	452 (97%)	12 (3%)	40	60	
1	W	464/466 (100%)	452 (97%)	12 (3%)	40	60	
1	X	464/466 (100%)	452 (97%)	12 (3%)	40	60	
1	Y	464/466 (100%)	452 (97%)	12 (3%)	40	60	
1	Z	464/466 (100%)	452 (97%)	12 (3%)	40	60	
1	a	464/466 (100%)	452 (97%)	12 (3%)	40	60	
1	b	464/466 (100%)	452 (97%)	12 (3%)	40	60	
1	c	464/466 (100%)	452 (97%)	12 (3%)	40	60	
1	d	464/466 (100%)	452 (97%)	12 (3%)	40	60	
1	e	464/466 (100%)	452 (97%)	12 (3%)	40	60	
1	f	464/466 (100%)	452 (97%)	12 (3%)	40	60	
1	g	464/466 (100%)	452 (97%)	12 (3%)	40	60	
1	h	464/466 (100%)	452 (97%)	12 (3%)	40	60	
1	i	464/466 (100%)	452 (97%)	12 (3%)	40	60	

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	j	464/466 (100%)	452 (97%)	12 (3%)	40	60
1	k	464/466 (100%)	452 (97%)	12 (3%)	40	60
1	l	464/466 (100%)	452 (97%)	12 (3%)	40	60
1	m	464/466 (100%)	452 (97%)	12 (3%)	40	60
1	n	464/466 (100%)	452 (97%)	12 (3%)	40	60
1	o	464/466 (100%)	452 (97%)	12 (3%)	40	60
1	p	464/466 (100%)	452 (97%)	12 (3%)	40	60
1	q	464/466 (100%)	452 (97%)	12 (3%)	40	60
1	r	464/466 (100%)	452 (97%)	12 (3%)	40	60
1	s	464/466 (100%)	452 (97%)	12 (3%)	40	60
1	t	464/466 (100%)	452 (97%)	12 (3%)	40	60
1	u	464/466 (100%)	452 (97%)	12 (3%)	40	60
1	v	464/466 (100%)	452 (97%)	12 (3%)	40	60
1	w	464/466 (100%)	452 (97%)	12 (3%)	40	60
1	x	464/466 (100%)	452 (97%)	12 (3%)	40	60
1	y	464/466 (100%)	452 (97%)	12 (3%)	40	60
1	z	464/466 (100%)	452 (97%)	12 (3%)	40	60
All	All	27840/27960 (100%)	27120 (97%)	720 (3%)	41	60

5 of 720 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	g	430	ASN
1	p	470	HIS
1	h	433	HIS
1	g	349	ILE
1	l	257	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 1178 such sidechains are listed below:

Mol	Chain	Res	Type
1	p	113	HIS
1	6	212	HIS
1	q	290	HIS
1	p	98	ASN

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Mol	Chain	Res	Type
1	v	113	HIS

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains [i](#)

There are no non-standard protein/DNA/RNA residues in this entry.

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

There are no ligands in this entry.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

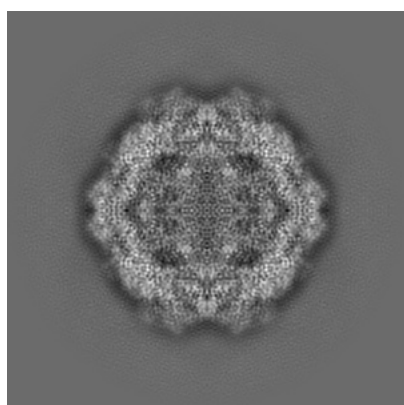
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-7301. These allow visual inspection of the internal detail of the map and identification of artifacts.

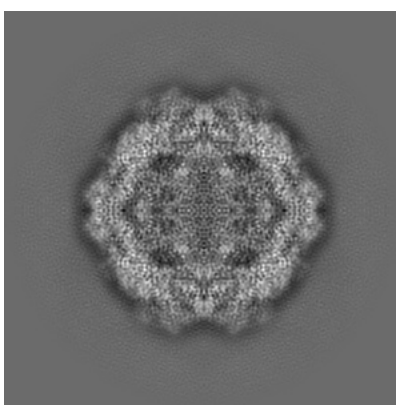
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

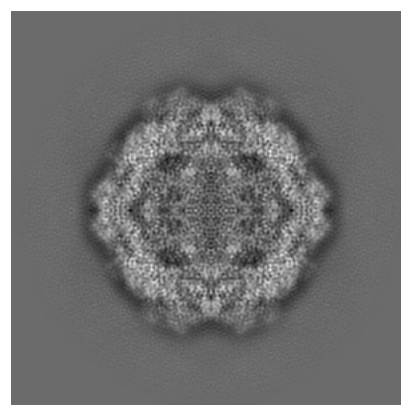
6.1.1 Primary map



X



Y

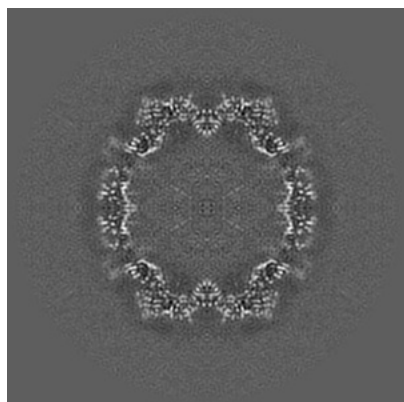


Z

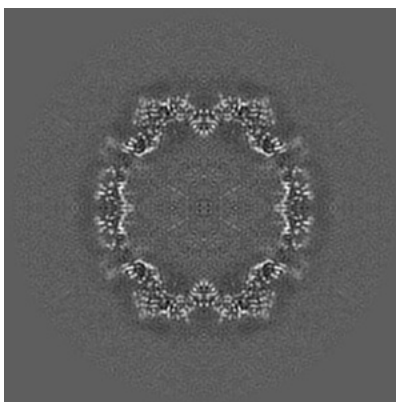
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

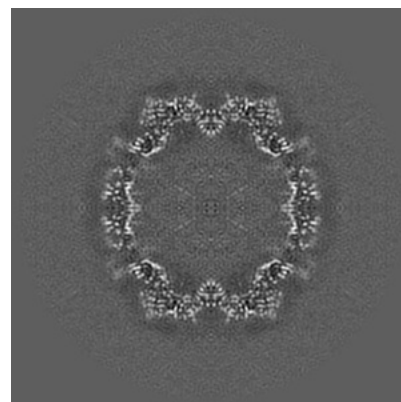
6.2.1 Primary map



X Index: 179



Y Index: 179

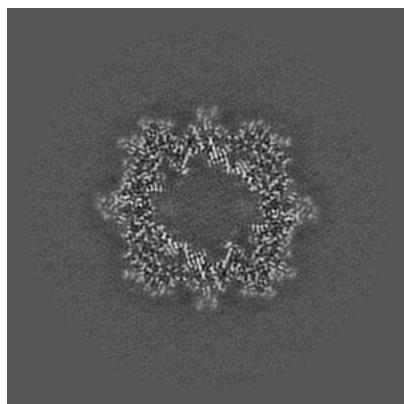


Z Index: 179

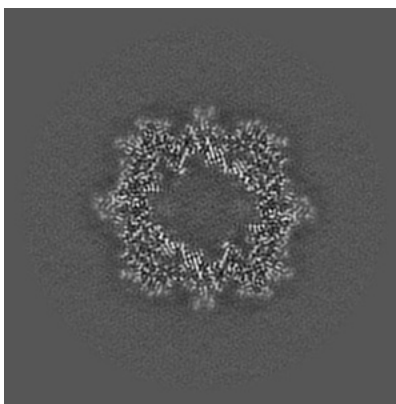
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

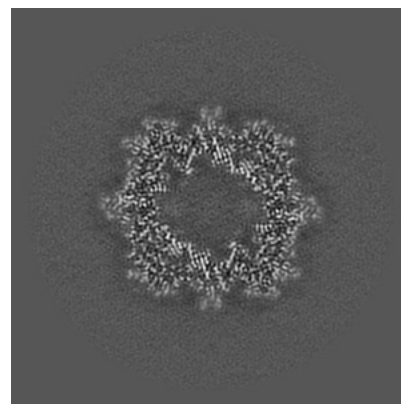
6.3.1 Primary map



X Index: 123



Y Index: 123

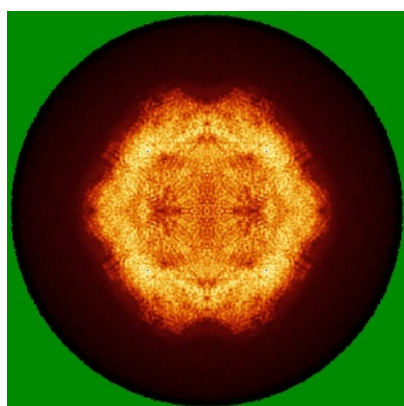


Z Index: 123

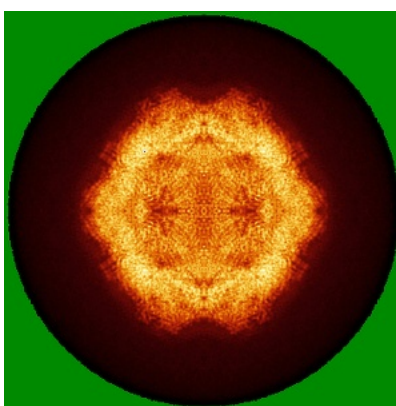
The images above show the largest variance slices of the map in three orthogonal directions.

6.4 Orthogonal standard-deviation projections (False-color) [i](#)

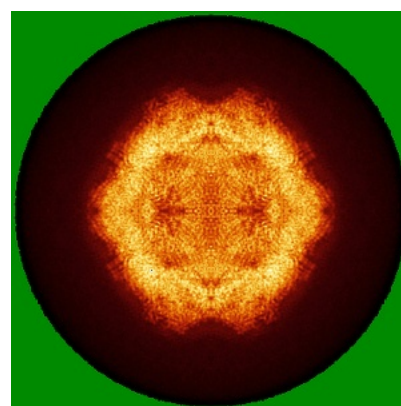
6.4.1 Primary map



X



Y

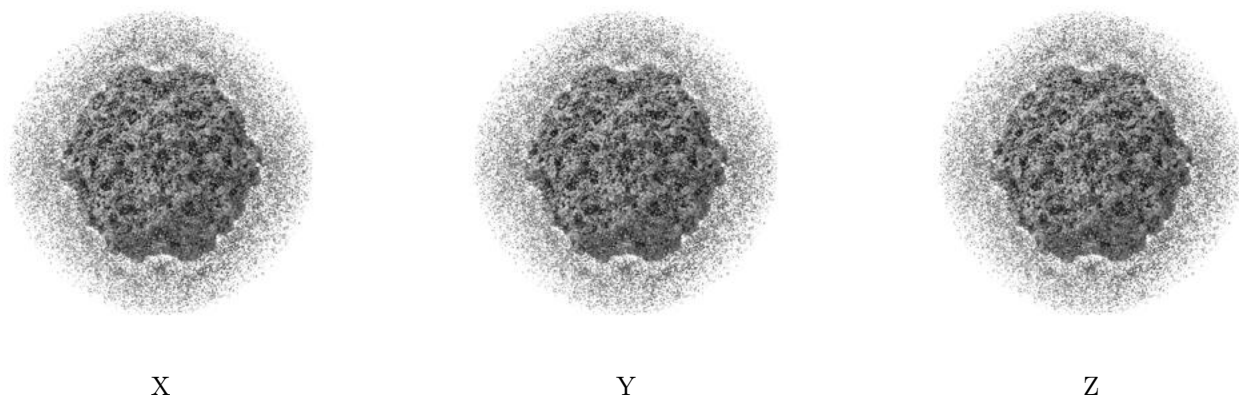


Z

The images above show the map standard deviation projections with false color in three orthogonal directions. Minimum values are shown in green, max in blue, and dark to light orange shades represent small to large values respectively.

6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 1.0. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

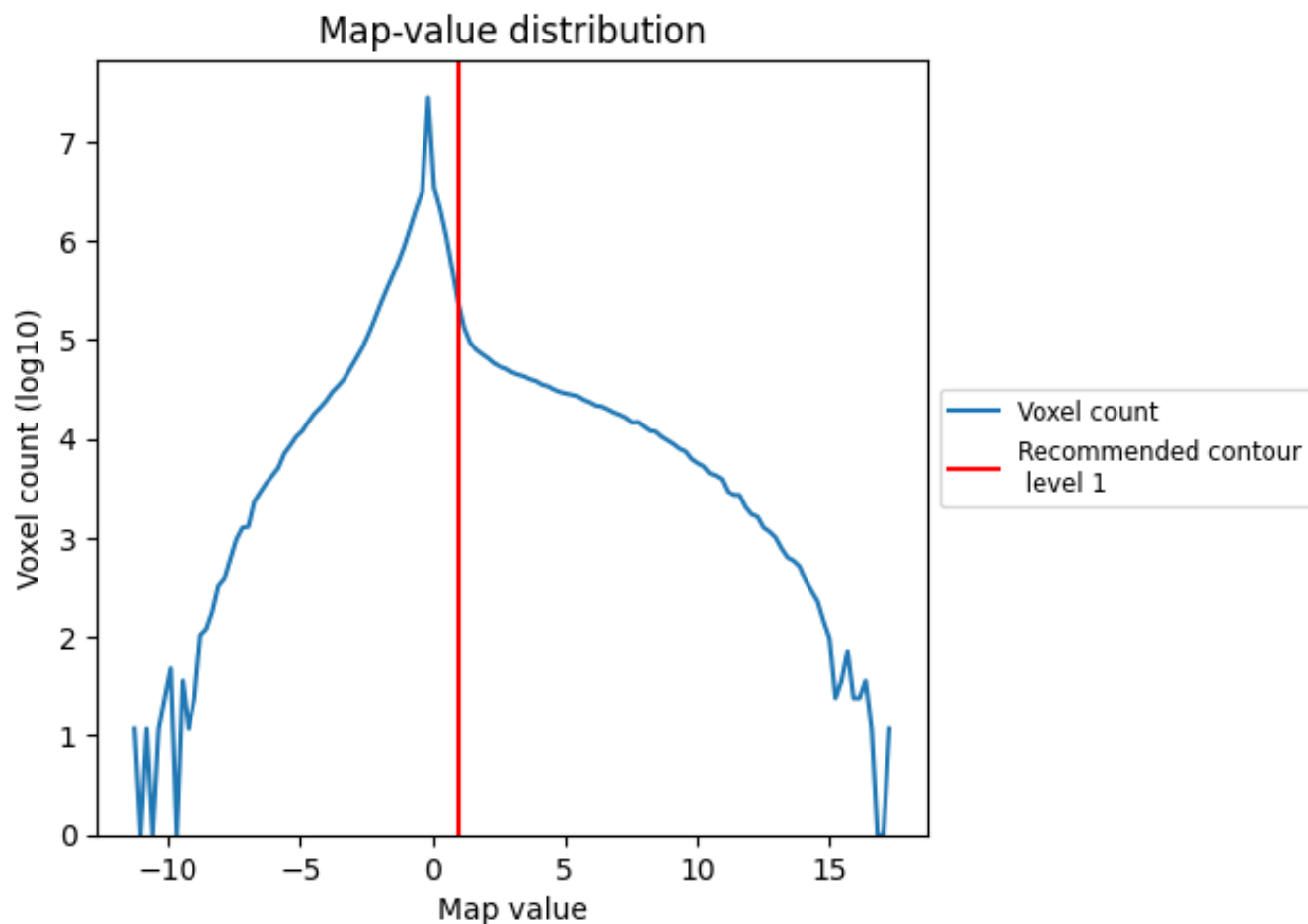
6.6 Mask visualisation [i](#)

This section was not generated. No masks/segmentation were deposited.

7 Map analysis [i](#)

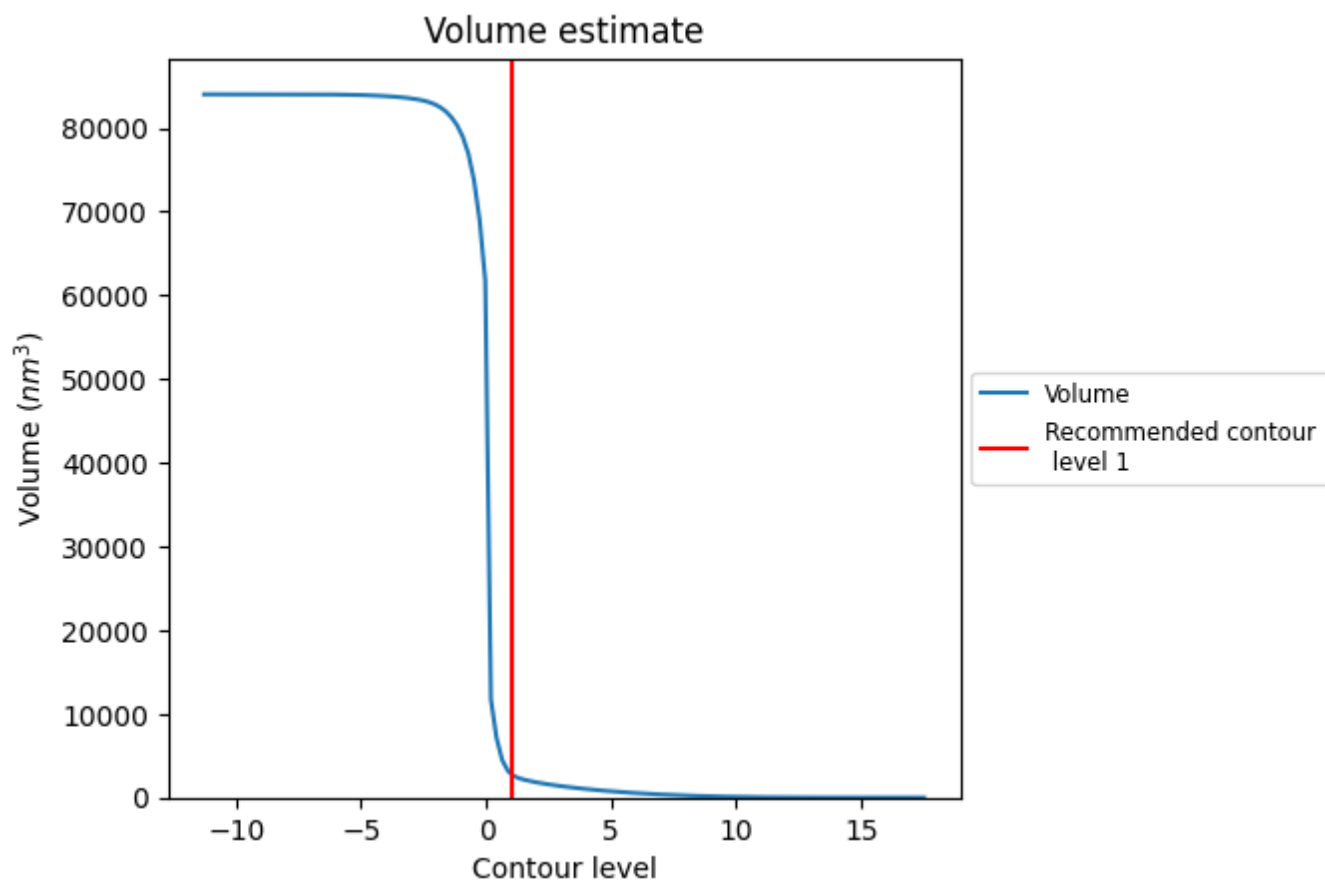
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution [i](#)



The map-value distribution is plotted in 128 intervals along the x-axis. The y-axis is logarithmic. A spike in this graph at zero usually indicates that the volume has been masked.

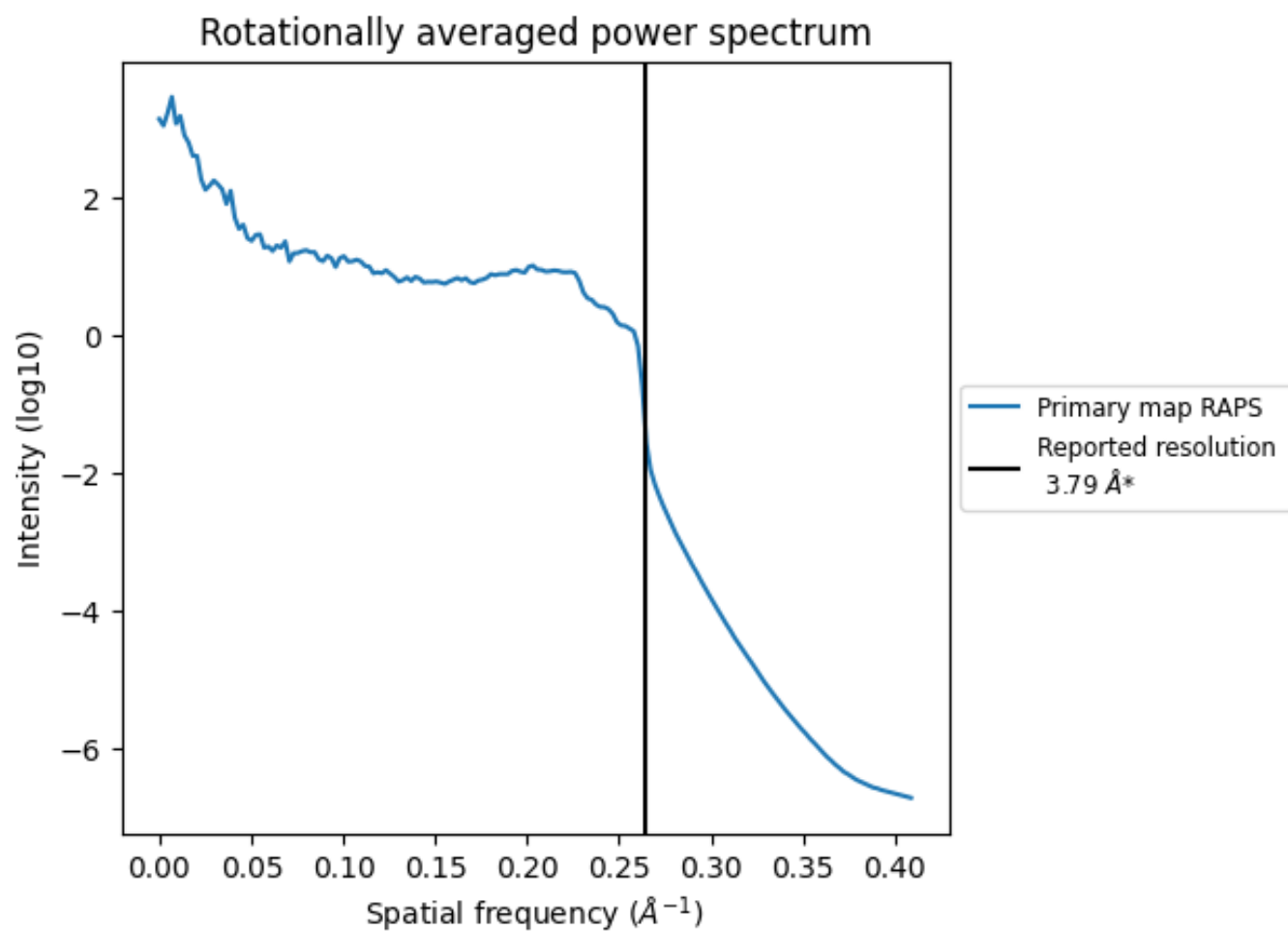
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 2859 nm³; this corresponds to an approximate mass of 2582 kDa.

The volume estimate graph shows how the enclosed volume varies with the contour level. The recommended contour level is shown as a vertical line and the intersection between the line and the curve gives the volume of the enclosed surface at the given level.

7.3 Rotationally averaged power spectrum ⓘ



*Reported resolution corresponds to spatial frequency of 0.264 Å⁻¹

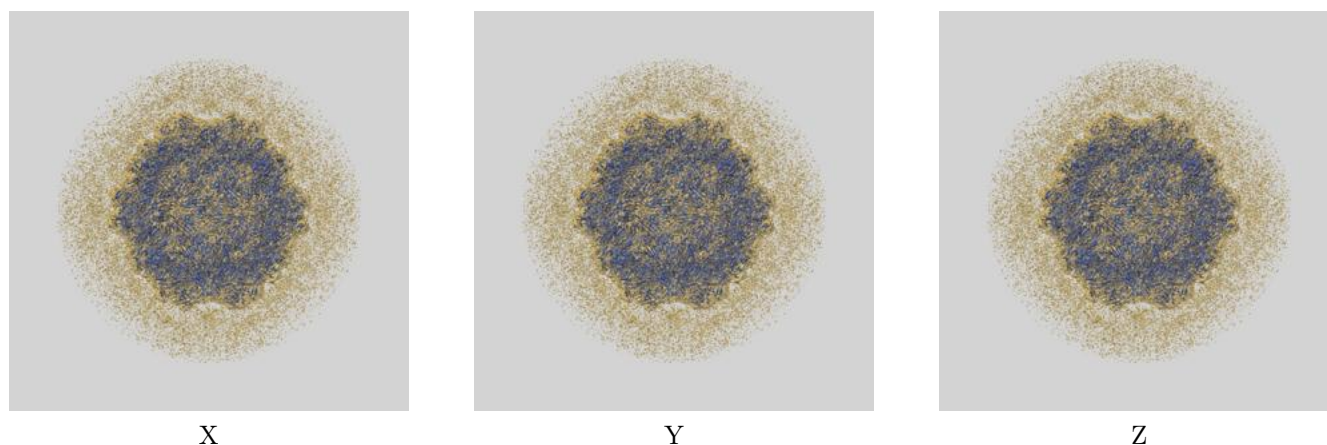
8 Fourier-Shell correlation

This section was not generated. No FSC curve or half-maps provided.

9 Map-model fit [i](#)

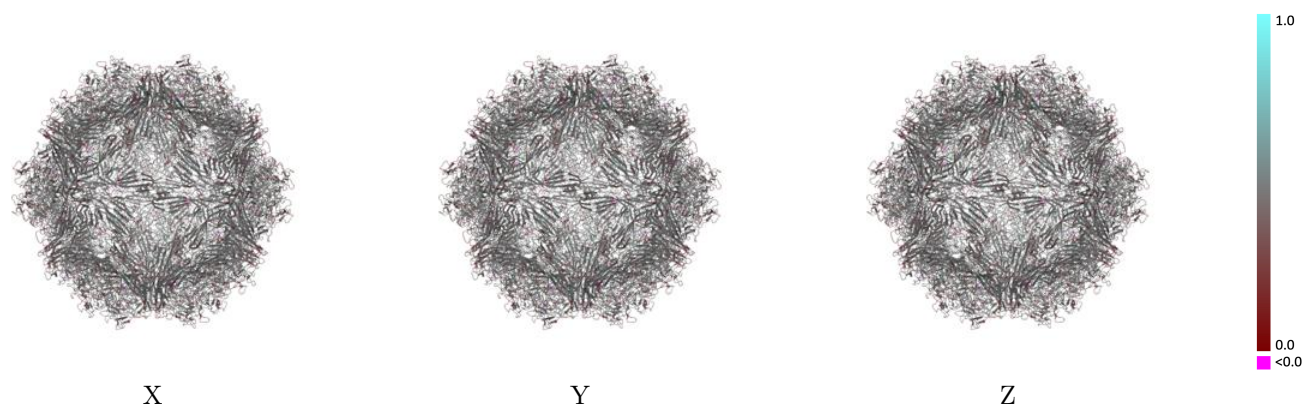
This section contains information regarding the fit between EMDB map EMD-7301 and PDB model 6BX0. Per-residue inclusion information can be found in [section 3](#) on [page 10](#).

9.1 Map-model overlay [i](#)



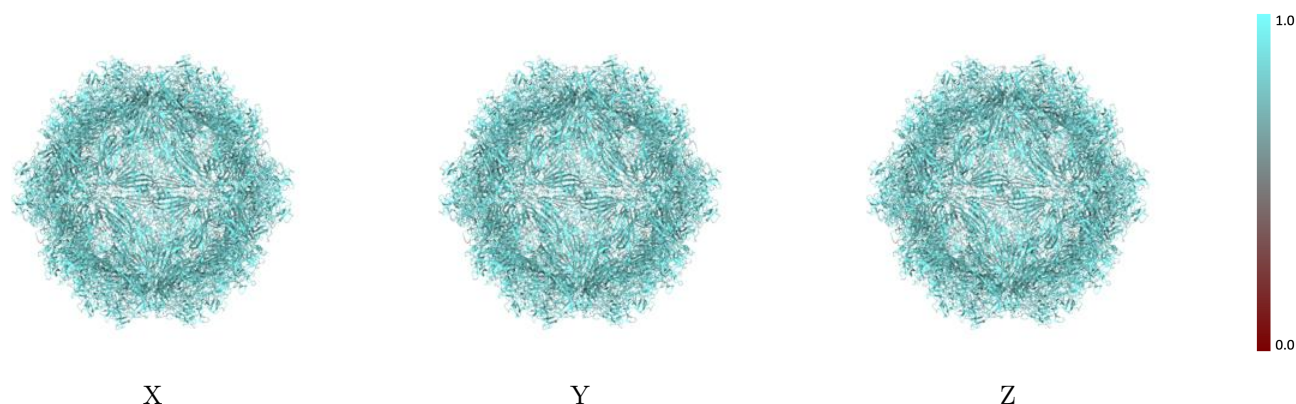
The images above show the 3D surface view of the map at the recommended contour level 1.0 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

9.2 Q-score mapped to coordinate model [i](#)



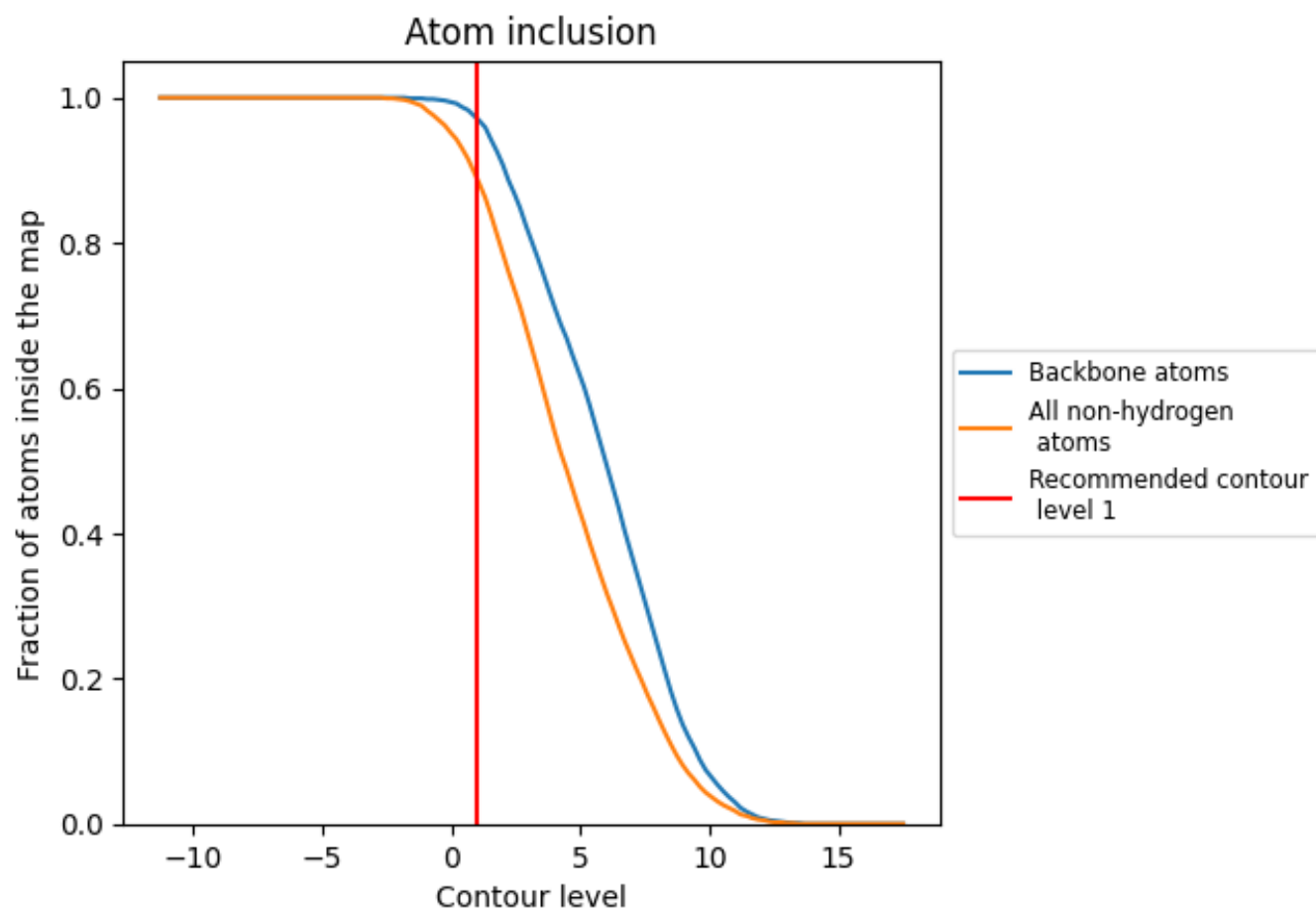
The images above show the model with each residue coloured according its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions at which atoms can be resolved. Low Q-score values may therefore be expected for many entries.

9.3 Atom inclusion mapped to coordinate model [i](#)



The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (1).

9.4 Atom inclusion [i](#)



At the recommended contour level, 97% of all backbone atoms, 89% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary ⓘ

The table lists the average atom inclusion at the recommended contour level (1) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.8890	 0.4470
0	 0.8880	 0.4450
1	 0.8890	 0.4460
2	 0.8890	 0.4470
3	 0.8890	 0.4480
4	 0.8880	 0.4450
5	 0.8890	 0.4450
6	 0.8880	 0.4450
7	 0.8880	 0.4460
A	 0.8900	 0.4470
B	 0.8890	 0.4470
C	 0.8880	 0.4480
D	 0.8880	 0.4450
E	 0.8880	 0.4440
F	 0.8890	 0.4460
G	 0.8890	 0.4470
H	 0.8890	 0.4470
I	 0.8890	 0.4460
J	 0.8880	 0.4460
K	 0.8880	 0.4460
L	 0.8890	 0.4470
M	 0.8880	 0.4460
N	 0.8880	 0.4450
O	 0.8880	 0.4450
P	 0.8880	 0.4470
Q	 0.8890	 0.4470
R	 0.8890	 0.4470
S	 0.8890	 0.4470
T	 0.8890	 0.4480
U	 0.8880	 0.4450
V	 0.8880	 0.4450
W	 0.8880	 0.4450
X	 0.8880	 0.4460
Y	 0.8890	 0.4480
Z	 0.8890	 0.4480



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Chain	Atom inclusion	Q-score
a	 0.8890	 0.4460
b	 0.8870	 0.4480
c	 0.8890	 0.4460
d	 0.8880	 0.4460
e	 0.8880	 0.4470
f	 0.8890	 0.4460
g	 0.8890	 0.4470
h	 0.8890	 0.4480
i	 0.8890	 0.4480
j	 0.8890	 0.4470
k	 0.8880	 0.4440
l	 0.8890	 0.4470
m	 0.8890	 0.4470
n	 0.8890	 0.4460
o	 0.8890	 0.4470
p	 0.8880	 0.4460
q	 0.8880	 0.4450
r	 0.8880	 0.4460
s	 0.8880	 0.4450
t	 0.8890	 0.4470
u	 0.8890	 0.4470
v	 0.8890	 0.4480
w	 0.8880	 0.4460
x	 0.8890	 0.4470
y	 0.8890	 0.4480
z	 0.8890	 0.4470